Supporting Information

On the Role of σ,π-Digold(I) Alkyne Complexes in Reactions of Enynes

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Supporting Information

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1. General Information

Unless otherwise stated, all reactions were carried out under argon atmosphere in solvents dried by passing through an activated alumina column on a PureSolv^{TM} solvent purification system (Innovative Technologies, Inc., MA). Thin layer chromatography was carried out using TLC aluminum sheets coated with 0.2 mm of silica gel (Merck Gf234). Chromatographic purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 µm) as the stationary phase. NMR spectra were recorded at 23 ºC on a Bruker Avance 300, 400 Ultrashield and Bruker Avance 500 Ultrashield apparatus. Chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane, using the residual protiosolvent or tetramethylsilane as reference. Coupling constants (*J*) are reported in hertz (*Hz*). Mass spectra were recorded on a Waters LCT Premier Spectrometer (ESI and APCI) or on an Autoflex Bruker Daltonics (MALDI and LDI). Melting points were determined using a MP70 melting point system Mettler Toledo melting point apparatus.

Unless otherwise stated, all reagents were purchased from commercial sources and used without further purification. Gold complexes were synthesized according to literature procedures.[1]

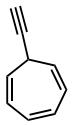
2. Experimental procedures

2.1 General procedure (A) for Au-catalyzed cyclization of enyne and 7-ethynylcyclohepta-1,3,5-triene substrates

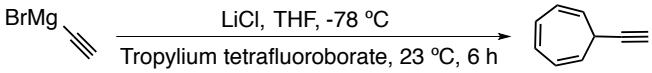
The substrate (1 equiv) was charged in a vial and dissolved in anhydrous CH_2Cl_2 (0.1 M solution) at 25 ºC, with no particular precautions taken to exclude air. Subsequently the gold (I) catalyst (5 mol%) was added in one portion at the same temperature and the reaction mixture stirred for 1 h in case of enynes and 1.5 hours in case of ethynyl cycloheptatriene. The reaction was quenched with a drop of Et_3N, the solvent was removed under reduced pressure (for volatile compounds, rotary evaporator bath at 19 ºC, ≥ 100 mbar). The crude product was purified by column chromatography on silica gel (see eluent below).

2.2 Experimental Procedures and compound Characterization for Organic Compounds

7-Ethynylcyclohepta-1,3,5-triene (11)



The title compound was prepared according to a literature procedure[2] by reaction between ethynyl magnesium bromide and tropylium tetrafluoroborate, and obtained as a colorless oil (439.6 mg, 3.780 mmol, 67%).



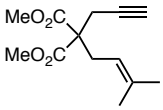
Previously dried LiCl (0.524 g, 12.360 mmol, 2.2 equiv) was placed in an oven-dried two-neck round-bottom flask under argon atmosphere. Dry THF (33 mL, 0.17 M) was added and the resulting suspension was cooled to -78 ºC. A solution of ethynyl magnesium bromide (0.5 M in THF, 22.48 mL, 12.240 mmol, 2 equiv) was added and the mixture was stirred 10 minutes at this temperature before addition of solid tropylium tetrafluoroborate (1.000 g, 5.620 mmol, 1 equiv) and stirring at this temperature for additional 10 min. Then the cooling bath was removed, and the mixture stirred at room temperature for 6 h. The reaction was quenched with a saturated aqueous solution of NH_4Cl and extracted with Et_2O (x3). The combined organic extracts were dried over $MgSO_4$ and the solvent was removed under reduced pressure (rotary evaporator bath at 19 ºC, ≥ 100 mbar). The crude residue was purified by column chromatography on silica gel eluting with pentane.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.66 (dd, *J* = 3.6, 2.7 Hz, 2H), 6.23-6.15 (m, 2H), 5.38-5.32 (m, 2H), 2.57-2.49 (m, 1H), 2.17 (d, *J* = 2.6 Hz, 1H).

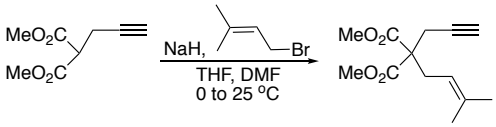
^{13}C NMR (101 MHz, $CDCl_3$) δ 131.16 (2xC), 125.10 (2xC), 122.95 (2xC), 85.76, 68.52, 31.51.

HRMS-APCI: calculated for C_9H_9 $[M+H]^+$: 117.0699; found = 117.0703.

Dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl)malonate (9)



The title compound was prepared from dimethyl propargylmalonate (3.0 g, 17.630 mmol), according to the procedure below, and obtained as a colorless oil (3.94 g, 16.54 mmol, 94%).



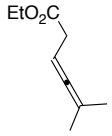
Dimethyl propargyl malonate (3.0 g, 17.630 mmol, 1 equiv) was added dropwise to a suspension of NaH (60 wt%, 550.0 mg, 22.92 mmol, 1.3 equiv) in a mixture of DMF (18 mL) and THF (18 mL) at 0 °C under Ar. The resulting mixture was stirred at 25 ºC for 15 min whereupon addition of 3,3-dimethylallyl bromide (3.15 g, 21.16 mmol, 1.2 equiv). The reaction mixture was stirred 15 h at 25 ºC. The reaction was quenched with water and extracted (x4) with Et_2O. The combined organic extracts were washed with brine (x4), dried over $MgSO_4$ and the solvent removed under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: 7:1 cyclohexane:ethyl acetate).

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.98-4.82 (m, 1H), 3.73 (s, 6H), 2.82-2.69 (m, 4H), 2.00 (t, J = 2.7 Hz, 1H), 1.70 (bs, 3H), 1.65 (bs, 3H).

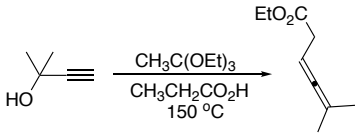
^{13}C NMR (126 MHz, $CDCl_3$) δ 170.63 (2xC), 137.09, 117.09, 79.42, 71.31, 57.31, 52.84 (2xC), 30.93, 26.20, 22.67, 18.08.

GC-MS-EI: calculated for $C_{13}H_{18}O_4$ $[M]^{\cdot+}$: 238.1; found = 238.1.

Ethyl 5-methylhexa-3,4-dienoate



The title compound was synthesized according to a literature procedure.[3]

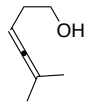


^{1}H NMR (300 MHz, $CDCl_3$) δ 5.15-5.00 (m, 1H), 4.14 (q, *J* = 7.1 Hz, 2H), 2.97 (d, *J* = 7.2 Hz, 2H), 1.69 (s, 3H), 1.68 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H).

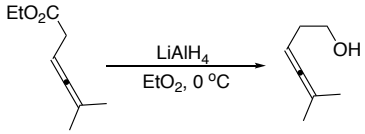
^{13}C NMR (126 MHz, $CDCl_3$) δ 203.09, 172.11, 96.49, 82.12, 60.73, 35.48, 20.55 (2xC), 14.36.

GC-MS-EI: calculated for $C_9H_{14}O_2$ $[M]^{\cdot+}$: 154.1; found = 154.1.

5-methylhexa-3,4-dien-1-ol



The title compound was prepared by reaction between ethyl 5-methylhexa-3,4-dienoate (600.0 mg, 3.89 mmol) and $LiAlH_4$, according to the procedure below, and obtained as a colorless oil (417.4 mg, 3.72 mmol, 96%).



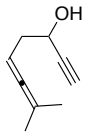
In a 100 mL schlenk flask under argon, $LiAlH_4$ (295 mg, 7.78 mmol, 2 equiv) was placed and suspended in anhydrous Et_2O (30 mL). It was cooled at 0°C, then a solution of ethyl 5-methylhexa-3,4-dienoate (600.0 mg, 3.89 mmol, 1 equiv) in anhydrous Et_2O (9mL) was added dropwise and the reaction mixture was stirred at this temperature for 1.5 h. The reaction was quenched with MeOH, then with a saturated aqueous solution of potassium sodium tartrate and extracted (x3) with Et_2O. The combined organic extracts were washed with the same saturated solution (x3), with brine (x1) and dried over $MgSO_4$. The solvent was removed under reduced pressure (rotary evaporator bath at 19 ºC, ≥ 100 mbar). The crude residue was purified by column chromatography on silica gel (eluent: 9:1 pentane:diethyl ether).

^{1}H NMR (300 MHz, $CDCl_3$) δ 5.10-4.80 (m, 1H), 3.68 (q, *J* = 6.0 Hz, 2H), 2.22 (q, *J*= 6.3 Hz, 2H), 1.70 (s, 3H), 1.69 (s, 3H), 1.56-1.51 (m, 1H).

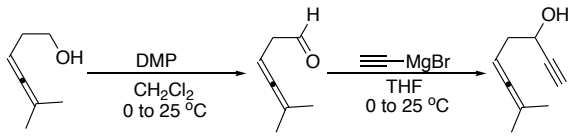
^{13}C NMR (75 MHz, $CDCl_3$) δ 202.67, 95.74, 85.13, 62.20, 32.60, 20.75 (2xC).

GC-MS-EI: calculated for $C_7H_{12}O$ $[M]^{\cdot+}$: 112.1; found =112.1.

7-methoxylocta-5,6-dien-1-yn-3-ol



The title compound was prepared via a two-step procedure starting from 5-methylhexa-3,4-dien-1-ol (562.2 mg, 5.01 mmol) according to the procedure below, and obtained as a colorless oil (118.0 mg, 0.87 mmol, 32%).



5-methylhexa-3,4-dien-1-ol (562.2 mg, 5.01 mmol, 1 equiv) was dissolved in CH_2Cl_2 (69 mL) and cooled to 0 °C whereupon addition of solid Dess-Martin periodinane (2551.0 mg, 6.01 mmol, 1.2 equiv). The reaction mixture was stirred at 25 °C for 1.5 h. It was quenched with water and extracted (x4) with Et_2O. The combined organic extracts were washed with a $NaHCO_3$ saturated solution (x1), brine (x1), dried over Na_2SO_4 and the solvent removed under reduced pressure (rotary evaporator bath at 19 ºC, ≥ 100 mbar). The crude was filtered through a silica pad and used directly without further purification.

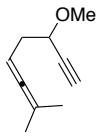
To a solution of the aldehyde (298.4 mg, 2.71 mmol, 1 equiv) in anhydrous THF (0.5 M in aldehyde) at 0 ºC under argon, was added a solution of ethynyl magnesium bromide (0.5 M in THF, 8.13 mL, 4.06 mmol, 1.5 equiv) dropwise and the resulting solution was stirred at 0 ºC for 15 min and warmed to 25 ºC for 1.5 h. The reaction was quenched with a saturated aqueous solution of NH_4Cl and extracted (x4) with Et_2O. The combined organic extracts were washed with brine (x1), dried over Na_2SO_4 and the solvent removed under reduced pressure (rotary evaporator bath at 19 ºC, ≥ 100 mbar). The crude product was purified by column chromatography on silica gel (eluent: 9:1 pentane:diethyl ether).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.07-4.91 (m, 1H), 4.44 (qd, *J* = 6.1, 2.1 Hz, 1H), 2.47 (d, *J* = 2.1 Hz, 1H), 2.43-2.34 (m, 2H), 2.01 (d, *J* = 6.2 Hz, 1H), 1.71 (s, 3H), 1.70 (s, 3H).

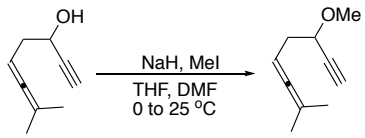
^{13}C NMR (75 MHz, $CDCl_3$) δ 203.64, 96.03, 84.48, 83.28, 73.10, 61.98, 37.87, 20.72 (2xC).

HRMS-APCI: calculated for $C_9H_{13}O$ $[M+H]^+$: 137.0961; found = 137.0961.

3-methoxy-7-methylocta-5,6-dien-1-yne



The title compound was prepared from 7-methoxylocta-5,6-dien-1-yn-3-ol (70 mg, 0.514 mmol) according to the procedure below, and obtained as a pale yellow oil (37 mg, 0.25 mmol, 48%).



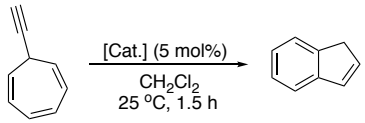
7-methoxylocta-5,6-dien-1-yn-3-ol (70 mg, 0.514 mmol, 1 equiv) dissolved in THF (4.4 mL) was added dropwise to a suspension of NaH (60 wt%, 30.8 mg, 0.771 mmol, 1.5 equiv) in DMF (0.7 mL) at 0 °C under argon. The resulting mixture was stirred at 0 ºC for 45 min whereupon addition of iodomethane (109 mg, 0.771 mmol, 1.5 equiv). The reaction mixture was stirred 4 h at 25 ºC. The reaction was quenched with water and extracted (x4) with Et_2O. The combined organic extracts were washed with brine (x4), dried over $MgSO_4$ and the solvent removed under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: 30:1 pentane:diethyl ether).

^{1}H NMR (500 MHz, $CDCl_3$) δ 5.03-4.93 (m, 1H), 3.99 (td, *J* = 6.6, 2.1 Hz, 1H), 3.42 (s, 3H), 2.45 (d, J = 2.0 Hz, 1H), 2.42-2.30 (m, 2H), 1.69 (s, 3 H), 1.69 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 203.16, 95.66, 83.93, 82.58, 73.99, 71.11, 56.59, 35.85, 20.69 (2xC).

HRMS-APCI: calculated for $C_{10}H_{15}O$ $[M+H]^+$: 151.1117; found = 151.1110.

1 *H*-indene (12)



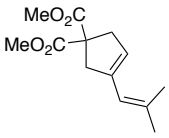
The title compound was prepared starting from 7-ethynylcyclohepta-1,3,5-triene (30 mg, 0.258 mmol) and the corresponding gold (I) catalyst (0.05 equiv) according to general procedure (**A**), and obtained as a colorless oil after purification by column chromatography on silica gel (eluent: pentane) (isolated yields, [*t*BuXPhosAuNCMe]BAr_4F (catalyst **A**), 22 mg, 0.189 mmol, 73%; [*i*PrAuNCMe]SbF_6 (catalyst **B**), 23 mg, 0.198 mmol, 77%).

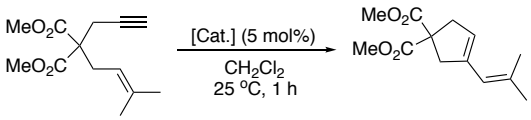
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.45 (m, 1H), 7.42 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.31-7.26 (m, 1H), 7.20 (td, *J* = 7.4, 1.2 Hz, 1H), 6.90 (dtd, *J* = 5.5, 1.9, 0.7 Hz, 1H), 6.57 (dt, *J* = 5.5, 2.0 Hz, 1H), 3.44-3.39 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.97, 143.81, 134.29, 132.20, 126.36, 124.67, 123.84, 121.09, 39.21.

GC-MS-EI: calculated for C_9H_8 $[M]^{\cdot+}$: 116.1; found = 116.1.

Dimethyl 3-(2-methylprop-1-en-1-yl)cyclopent-3-ene-1,1-dicarboxylate (10a)





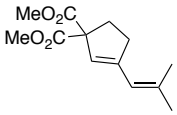
The title compound was prepared starting from dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl)malonate (30 mg, 0.126 mmol) and the corresponding gold (I) catalyst (0.05 equiv) according to general procedure (**A**), and obtained after purification by column chromatography on silica gel (eluent: 10:1 cyclohexane:AcOEt) as a colorless oil. (Isolated yield with [*i*PrAuNCMe]SbF_6 (catalyst **B**), 98%, 29.3 mg, 0.123 mmol)

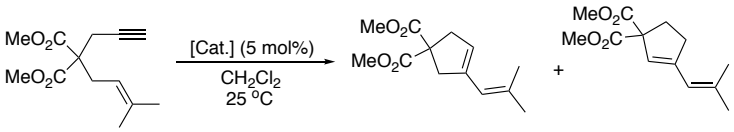
^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 (bs, 1H), 5.39 (bs, 1H), 3.74 (s, 6H), 3.22-3.16 (m, 2H), 3.05 (bs, 2H), 1.82 (s, 3H), 1.78 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.78 (2xC), 138.90, 135.81, 124.57, 120.79, 59.50, 52.97 (2xC), 43.44, 40.45, 27.41, 19.99.

GC-MS-EI: calculated for $C_{13}H_{18}O_4$ $[M]^{\cdot+}$: 238.1; found = 238.1.

Dimethyl 3-(2-methylprop-1-en-1-yl)cyclopent-2-ene-1,1-dicarboxylate (10b)





The title compound was prepared starting from dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl)malonate and the corresponding gold (I) catalyst (0.05 equiv) according to general procedure (**A**), stirring the reaction for longer times (*ca.* 17 h) and obtained after purification by column chromatography on silica gel (eluent: 10:1 cyclohexane:AcOEt) as an inseparable mixture with dimethyl 3-(2-methylprop-1-en-1-yl)cyclopent-3-ene-1,1-dicarboxylate; colorless oil.

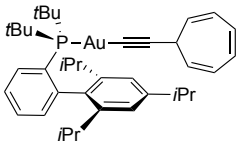
^{1}H NMR (500 MHz, $CDCl_3$) δ 5.80 (bs, 1H), 5.59 (bs, 1H), 3.72 (s, 6H), 2.70-2.62 (m, 2H), 2.51-2.44 (m, 2H), 1.84 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.14 (2xC), 146.26, 138.16, 124.99, 120.82, 66.12, 52.79 (2xC), 34.91, 32.27, 27.54, 20.05.

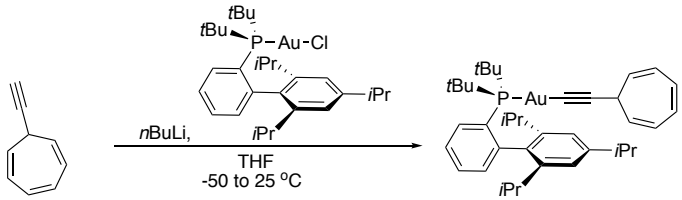
GC-MS-EI: calculated for $C_{13}H_{18}O_4$ $[M]^{\cdot+}$: 238.1; found = 238.1.

2.3 Experimental Procedures and compound Characterization for Gold Acetylides and Digold complexes

[(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine](2-cyclohepta-2,4,6-trien-1-ylethynyl)gold (15)



The title compound was prepared according to the procedure below, and obtained as a beige solid (42.2 mg, 0.057 mmol, 75%).



An oven-dried schlenk or vial under argon atmosphere was charged with 7-ethynylcyclohepta-1,3,5-triene (17.68 mg, 0.152 mmol, 2 equiv) in anhydrous THF (0.8 mL) the resulting solution was cooled to -50 ºC before adding *n*BuLi (2.5 M in hexanes, 0.067 mL, 0.167 mmol, 2.2 equiv) dissolved in 0.2 mL anhydrous THF and stirring for 30 min at this temperature. Chloro[(2′,4′,6′-triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine]gold(I) (50 mg, 0.076 mmol, 1 equiv) was dissolved in anhydrous THF (2 mL) under Ar and added to the reaction mixture. The cooling bath was maintained for 15 min and then the mixture was stirred at 25 ºC for 10 h. The crude was concentrated, dissolved in CH_2Cl_2 and filtered through cotton and Teflon 0.22. The solvent was removed and the resulting solid was washed with pentane.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (td, *J* = 7.4, 1.6 Hz, 1H), 7.50-7.40 (m, 2H), 7.32-7.26 (m, 1H), 7.10 (s, 2H), 6.59 (t, *J* = 3.1 Hz, 2H), 6.12-6.04 (m, 2H), 5.39 (dd, *J* = 9.1 5.4 Hz, 2H), 2.97 (hept, *J* = 7.0 Hz, 1H), 2.44-2.37 (m, 1H), 2.39-2.32 (m, 2H), 1.42 (d, *J* = 14.7 Hz, 18H), 1.34 (d, *J* = 6.8 Hz, 6H), 1.32 (d, *J* = 6.9 Hz, 6H), 0.92 (d, *J* = 6.6 Hz, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.39 (CqAr), 148.66 (d, *J* (^{13}C-^{31}P) = 15.7 Hz (CqAr-P), 145.68 (3xC, CqAr*i*Pr), 135.85 (d, *J* (^{13}C-^{31}P) = 4.9 Hz (CqAr)), 135.46 (d, *J* (^{13}C-^{31}P) = 1.4 Hz (CHAr)), 134.84 (d, *J* (^{13}C-^{31}P) = 7.8 Hz (CHAr)), 130.64 (2xC, CHT), 130.02-129.61 (m, CHAr), 126.93 (2xC, CHT), 126.24 (d, *J* (^{13}C-^{31}P) = 5.9 Hz (CHAr)), 123.24 (2xC, CHT), 122.66 (Cq), 121.97 (2xC, CHArorto*i*Pr), 121.60 (Cq), 102.88 (d, *J* (^{13}C-^{31}P) = 24.1 Hz (Cq*t*Bu)), 38.17 (d, *J* (^{13}C-^{31}P) = 22.8 Hz (Cq*t*Bu)), 34.03 (CH*i*Pr), 33.42 (d, *J* (^{13}C-^{31}P) = 2.3 Hz (CH-CHT), 31.58 (d, *J* (^{13}C-^{31}P) = 6.8 Hz (6xC, CH_3*t*Bu), 31.03 (2xC, CH*i*Pr), 26.47 (2xC, CH_3*i*Pr), 24.35 (2xC, CH_3*i*Pr), 23.15 (2xC, CH_3*i*Pr).

^{31}P{^{1}H} NMR (126 MHz, $CDCl_3$) δ 67.23.

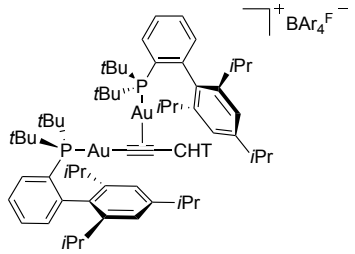
IR (neat) 2960, 2866, 1461, 1367, 1265, 1167, 772, 745, 707 cm^{-1}.

HRMS-ESI: calculated for $C_{38}H_{52}AuNaP$ $[M+Na]^+$: 759.3365; found = 759.3393. Anal. calcd. For $C_{38}H_{52}AuP$: C, 61.95; H, 7.11; found: C, 62.23; H, 6.85.

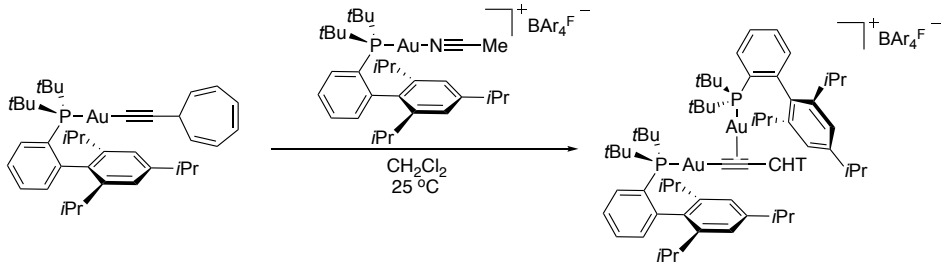
Melting point: 190-197 °C decomposition.

Structure confirmed by X-ray crystallography: CCDC 1572067.

{[(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine](2- cyclohepta-2,4,6-trien-1-ylethynyl)gold}[(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine] gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (16)



The title compound was prepared according to the procedure below, and obtained as a beige solid (85 mg, 0.038 mmol, 71%).



To a solution of [(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine](2-cyclohepta-2,4,6-trien-1-ylethynyl)gold (39.9 mg, 0.054 mmol, 1 equiv) in CH_2Cl_2 (5.4 mL) was added (acetonitrile)[(2′,4′,6′-triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine]gold(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (83 mg, 0.054 mmol, 1 equiv) solid and the mixture was stirred for 1 h. The crude was concentrated, the resulting solid redissolved in CH_2Cl_2, then filtered through Celite, through Teflon 0.22 and concentrated. The solid was washed with pentane.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (td, *J* = 7.7, 1.9 Hz, 2H), 7.73-7.71 (m, 8H), 7.52 (s, 4H), 7.51-7.46 (m, 4H), 7.22 (ddd, *J* = 7.1, 4.7, 2.0 Hz, 2H), 6.90 (s, 4H), 6.71 (t, *J* = 3.1 Hz, 2H), 6.27-6.17 (m, 2H), 5.13 (dd, *J* = 9.0, 5.4 Hz, 2H), 2.74 (hept, *J* = 6.6 Hz, 2H), 2.45-2.36 (m, 1H), 2.30 (hept, *J* = 6.6 Hz, 4H), 1.39 (d, *J* = 15.6 Hz, 36H), 1.20 (d, *J* = 6.9 Hz, 12H), 1.17 (d, *J* = 6.8 Hz, 12H), 0.87 (d, *J* = 6.6 Hz, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.87 (q, *J* (^{13}C-^{11}B) = 50.5 Hz (4xC, Cq)), 149.55 (2xC, CqAr), 147.57 (d, *J* (^{13}C-^{31}P) = 14.3 Hz (2xC, CqAr-P), 146.64 (6xC, CqAr*i*Pr), 135.75 (d, *J* (^{13}C-^{31}P) = 5.5 Hz (2xC, CqAr)), 134.97 (2xC, CHAr), 134.96 (8xC, CHArorto BAr_4F), 134.95 (2xC, CHAr), 131.51 (2xC, CHT), 131.06 (2xC, CHAr), 129.67-128.32 (m, 8xC, CqAr), 127.17 (d, *J* (^{13}C-^{31}P) = 6.2 Hz (2xC, CHAr)), 126.78 (Cq), 125.39 (2xC, CHT), 124.71 (q, *J* (^{13}C-^{19}F) = 272.6 Hz (8xC, Cq)), 122.65 (2xC, CHT), 122.04 (Cq), 121.77 (4xC, CHArorto*i*Pr), 117.72-117.44 (m, 4xC, CHArpara BAr_4F), 38.94 (d, *J* (^{13}C-^{31}P) = 24.7 Hz (4xC, Cq*t*Bu)), 34.57 (CH-CHT), 33.58 (2xC, CH*i*Pr), 31.49 (d, *J* (^{13}C-^{31}P) = 6.7 Hz (12xC, CH_3*t*Bu), 30.93 (4xC, CH*i*Pr), 26.15 (4xC, CH_3*i*Pr), 24.16 (4xC, CH_3*i*Pr), 23.62 (4xC, CH_3*i*Pr).

^{31}P{^{1}H} NMR (202 MHz, $CDCl_3$) δ 64.71.

^{19}F{^{1}H} NMR (376 MHz, $CDCl_3$) δ -62.52.

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -6.67.

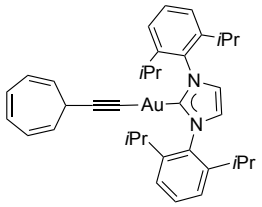
IR (neat) 2960, 2866, 1461, 1367, 1265, 1167, 772, 745, 707 cm^{-1}.

HRMS-ESI: calculated for $C_{67}H_{97}Au_2P_2$ $[M-C_{32}H_{12}BF_{24}]^+$: 1357.6391; found = 1357.6408. Anal. calcd. For $C_{99}H_{109}Au_2BF_{24}P_2$: C, 53.52; H, 4.95; found: C, 53.10; H, 4.90.

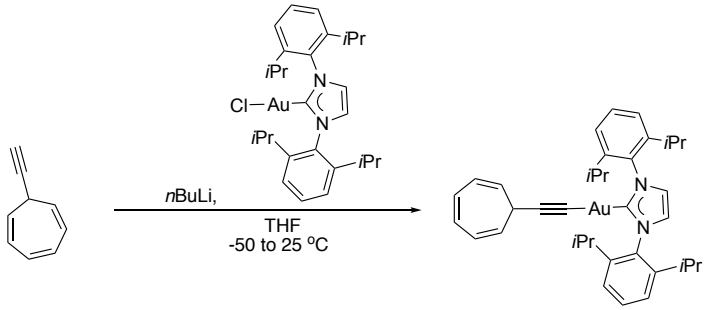
Melting point: 203-205 °C.

Structure confirmed by X-ray crystallography: CCDC 1572069.

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl]gold (17)



The title compound was prepared according to the procedure below, and obtained as a beige solid (51.0 mg, 0.073 mmol, 85%).



An oven-dried schlenk or vial under argon atmosphere was charged with 7-ethynylcyclohepta-1,3,5-triene (19.83 mg, 0.171 mmol, 2 equiv) in anhydrous THF (0.8 mL) the resulting solution was cooled to -50 ºC before adding *n*BuLi (2.5 M in hexanes, 0.075 mL, 0.188 mmol, 2.2 equiv) dissolved in 0.2 mL anhydrous THF and stirring for 30 min at this temperature. Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (53 mg, 0.085 mmol, 1 equiv) was dissolved in anhydrous THF (2.4 mL) under Ar and added to the reaction mixture. The cooling bath was maintained for 15 min and then the mixture was stirred at 25 ºC for 10 h. The crude was concentrated, dissolved in CH_2Cl_2 and filtered through cotton and Teflon 0.22. The solvent was removed and the resulting solid was washed with pentane.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (t, *J* = 7.8 Hz, 2H), 7.28 (d, *J* = 7.8 Hz, 4H), 7.10 (s, 2H), 6.51 (t, *J* = 3.1 Hz, 2H), 6.02-5.96 (m, 2H), 5.28 (dd, *J* = 9.1, 5.4 Hz, 2H), 2.61 (hept, *J* = 6.8 Hz, 4H), 2.44-2.38 (m, 1H), 1.37 (d, *J* = 6.9 Hz, 12 H), 1.20 (d, *J* = 6.9 Hz, 12H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 191.46 (C carbene), 145.76 (4xC, CqAr*i*Pr), 134.55 (2xC, CqArN), 130.59 (2xC, CHArpara), 130.56 (2xC, CHT), 126.46 (2xC, CHT), 124.30 (4xC, CHArmeta), 123.28 (2xC, CHT) overlapped with (2xC, CH imidazole), 116.09, 105.44, 33.26 (CH, CHT), 28.95 (4xC), 24.74 (4xC), 24.19 (4xC).

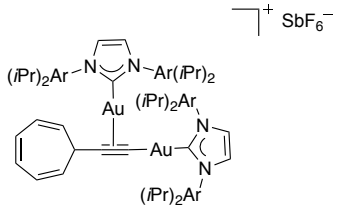
IR (neat) 3155, 2961, 2926, 2867, 1468, 1413, 1385, 1270, 805, 748, 706 cm^{-1}.

HRMS-ESI: calculated for $C_{36}H_{44}AuN_2$ $[M+H]^+$: 701.3165; found = 701.3159.

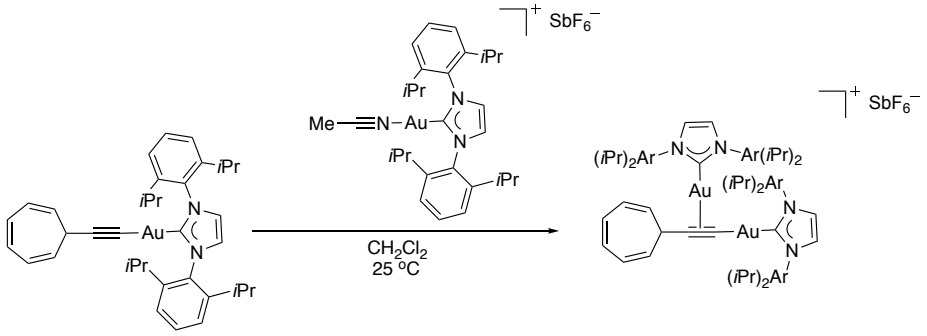
Melting point: 169-177 °C decomposition.

Structure confirmed by X-ray crystallography: CCDC 1572073.

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (18a)



The title compound was prepared according to the procedure below, and obtained as a beige solid (94 mg, 0.073 mmol, 100%).



To a solution of [(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl]gold (51 mg, 0.073 mmol, 1 equiv) in CH_2Cl_2 (7.2 mL) was added acetonitrile[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) hexafluoroantimonate (62.8 mg, 0.073 mmol, 1 equiv) solid and the mixture was stirred for 1 h. The crude was concentrated, the resulting solid redissolved in CH_2Cl_2, then filtered through Celite, through Teflon 0.22 and concentrated. The solid was washed with pentane.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (t, J = 7.8 Hz, 4H), 7.24 (s, 8H), 7.23 (s, 4H), 6.46 (t, J = 3.1 Hz, 2H), 5.95-5.86 (m, 2H), 4.53 (dd, J = 9.1, 5.6 Hz, 2H), 2.44 (hept, J = 6.7 Hz, 8H), 2.26 (tt, J = 5.7, 1.2 Hz, 1H), 1.18 (d, J = 6.9 Hz, 24H), 1.07 (d, J = 6.9 Hz, 24H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 183.07 (2xC, C carbene), 145.65 (8xC, CqAr*i*Pr), 133.78 (4xC, CqArN), 130.96 (2xC, CHT), 130.89 (4xC, CHArpara), 124.94 (2xC, CHT), 124.34 (8xC, CHArmeta), 124.28 (4xC, CH imidazole), 122.31 (2xC, CHT), 119.78, 115.11, 33.70 (CH, CHT), 28.83 (8xC), 24.71 (8xC), 24.05 (8xC).

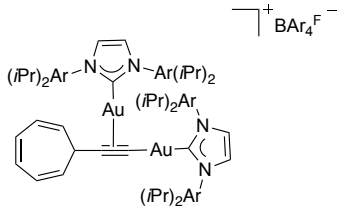
IR (neat) 3171, 2961, 2927, 2870, 1555, 1459, 1418, 1386, 1329, 1215, 1060, 804, 758, 705, 655 cm^{-1}.

HRMS-ESI: calculated for $C_{63}H_{79}Au_2N_4$ $[M-SbF_6]^+$: 1285.5631; found = 1285.5613. Anal. calcd. For $C_{63}H_{79}Au_2F_6N_4Sb$: C, 49.72; H, 5.23; N, 3.68; found: C, 50.05; H, 5.22; N, 3.69.

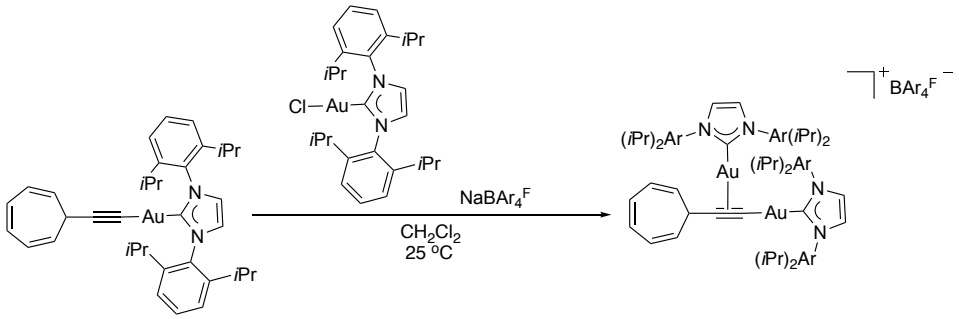
Melting point: 170-176 °C decomposition.

Structure confirmed by X-ray crystallography: CCDC 1572065.

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (18b)



The title compound was prepared according to the procedure below, and obtained as a beige solid (28.4 mg, 0.013 mmol, 93%).



Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (8.86 mg, 0.014 mmol, 1 equiv) and [(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl]gold (10 mg, 0.014 mmol, 1 equiv) were dissolved in CH_2Cl_2 (1.4 mL). Then sodium tetrakis[3,5-bis(trifluoromethyl)phenyl] borate (12.65 mg, 0.014 mmol, 1 equiv) solid was added and the reaction mixture was stirred for 30 min. The crude was filtered through Celite, through Teflon 0.22 and concentrated. The resulting solid was washed with pentane.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73-7.68 (m, 8H), 7.52 (bs, 4H), 7.49 (t, *J* = 7.8 Hz, 4H), 7.24 (d, *J* = 7.8 Hz, 8H), 7.16 (s, 4H), 6.48-6.45 (m, 2H), 5.95-5.86 (m, 2H), 4.53 (dd, *J* = 8.9, 5.6 Hz, 2H), 2.41 (hept, *J* = 6.8 Hz, 8H), 2.26 (ddd, *J* = 6.8, 5.6, 1.8 Hz, 1H), 1.16 (d, *J* = 6.9 Hz, 24H), 1.08 (d, *J* = 6.9 Hz, 24H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 183.51 (2xC, C carbene), 161.83 (q, *J* (^{13}C-^{11}B) = 50.5 Hz (4xC, Cq)), 145.57 (8xC, CqAr*i*Pr), 134.96 (8xC, CHArorto BAr_4F), 133.62 (4xC, CqArN), 131.04 (4xC, CHArpara), 130.99 (2xC, CHT), 128.98 (dddd, *J* (^{13}C-^{19}F) = 34.3, 31.4, 27.1, 4.1 Hz (8xC, Cq)), 124.72 (q, *J* (^{13}C-^{19}F) = 272.5 Hz (8xC, Cq)), 125.04 (2xC, CHT), 124.43 (8xC, CHArmeta), 123.92 (4xC, CH imidazole), 122.08 (2xC, CHT), 119.52, 117.57 (dt, *J* (^{13}C-^{19}F) = 7.5, 3.7 Hz (4xC, CHArpara BAr_4F)), 115.46, 33.70 (CH, CHT), 28.88 (8xC), 24.67 (8xC), 24.00 (8xC).

^{19}F{^{1}H} NMR (376 MHz, $CDCl_3$) δ -62.55.

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -6.68.

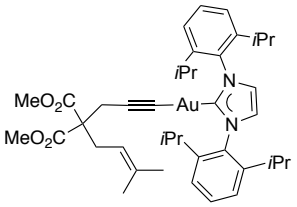
IR (neat) 2964, 2925, 2851, 1461, 1353, 1274, 1119, 886, 803, 712, 681 cm^{-1}.

HRMS-ESI: calculated for $C_{63}H_{79}Au_2N_4$ $[M-C_{32}H_{12}BF_{24}]^+$: 1285.5631; found = 1285.5650. Anal. calcd. For $C_{95}H_{91}Au_2BF_{24}N_4$: C, 53.08; H, 4.27; N, 2.61; found: C, 53.08; H, 4.30; N, 2.63.

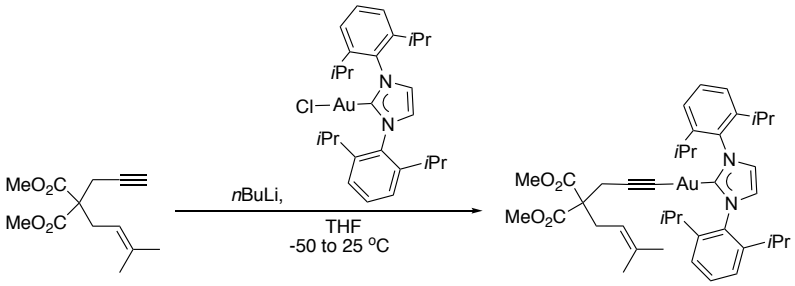
Melting point: 52-55 °C.

Structure confirmed by X-ray crystallography: CCDC 1572072.

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)]gold (13)



The title compound was prepared according to the procedure below, and obtained as a beige solid (55.7 mg, 0.068 mmol, 84%).



An oven-dried schlenk or vial under argon atmosphere was charged with dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl)malonate (28.8 mg, 0.121 mmol, 1.5 equiv) in anhydrous THF (0.8 mL) the resulting solution was cooled to -50 ºC before adding *n*BuLi (2.5 M in hexanes, 0.058 mL, 0.145 mmol, 1.8 equiv) dissolved in 0.2 mL anhydrous THF and stirring for 30 min at this temperature. Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (50 mg, 0.081 mmol, 1 equiv) was dissolved in anhydrous THF (2.2 mL) under Ar and added to the reaction mixture. The cooling bath was maintained for 15 min and then the mixture was stirred at 25 ºC for 10 h. The crude was concentrated, dissolved in CH_2Cl_2 and filtered through cotton and Teflon 0.22. The solvent was removed and the resulting solid was washed with pentane.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (t, *J* = 7.8 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 4H), 7.10 (s, 2H), 4.87-4.77 (m, 1H), 3.56 (s, 6H), 2.71 (s, 2H), 2.68 (d, *J* = 7.7 Hz, 2H), 2.56 (hept, *J* = 6.8 Hz, 4H), 1.60 (s, 3H), 1.49 (s, 3H), 1.34 (d, *J* = 6.9 Hz, 12H), 1.20 (d, *J* = 6.9 Hz, 12H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.70 (C carbene), 171.44 (2xC, COOMe), 145.81 (4xC, CqAr*i*Pr), 135.83 (Cq enyne), 134.44 (2xC, CqArN), 130.44 (2xC, CHArpara), 124.17 (4xC, CHArmeta), 123.07 (2xC, CH imidazole), 119.81, 118.29 (CH enyne), 98.42, 58.47 (Cq enyne), 52.3 (2xC, $COOCH_3$), 30.87 (CH_2 enyne), 28.92 (4xC), 26.17 (CH_3 enyne), 24.61 (4xC), 24.47 (CH_2 enyne), 24.16 (4xC), 18.14 (CH_3 enyne).

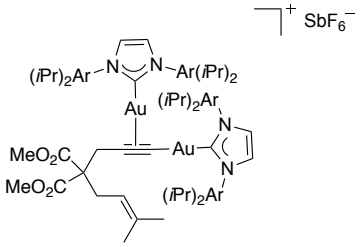
IR (neat) 2961, 2927, 2868, 1734, 1458, 1287, 1222, 1180, 1058, 803, 729 cm^{-1}.

HRMS-ESI: calculated for $C_{40}H_{54}AuN_2O_4$ $[M+H]^+$: 823.3744; found = 823.3741.

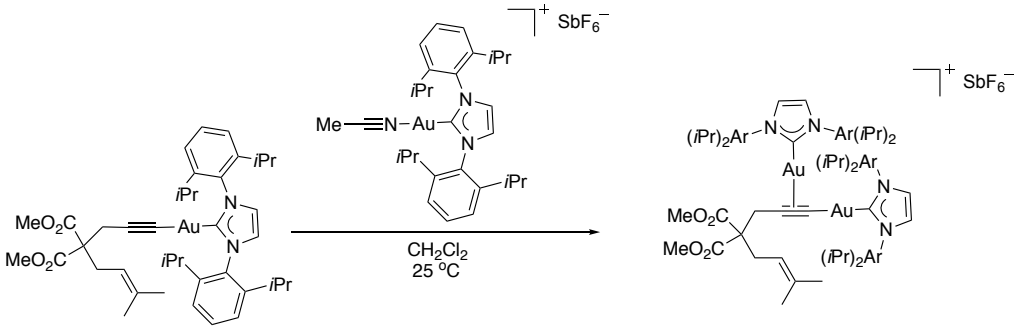
Melting point: 110.7-111.0 °C.

Structure confirmed by X-ray crystallography: CCDC 1572070.

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (14a)



The title compound was prepared according to the procedure below, and obtained as a beige solid (13.2 mg, 0.0094 mmol, 43%).



To a solution of [(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)]gold (18 mg, 0.022 mmol, 1 equiv) in CH_2Cl_2 (1.2 mL) was added acetonitrile[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) hexafluoroantimonate (18.86 mg, 0.022 mmol, 1 equiv) solid and the mixture was stirred for 1 h. The crude was concentrated, the resulting solid redissolved in CH_2Cl_2, then filtered through Celite, through Teflon 0.22 and concentrated. The solid was washed with pentane.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (t, *J* = 7.8 Hz, 4H), 7.26 (s, 4H), 7.24 (d, *J* = 4.3 Hz, 8H), 4.54 (t, *J* = 8.0 Hz, 1H), 3.44 (s, 6H), 2.42 (hept, *J* = 6.8 Hz, 8H), 2.28 (s, 2H), 2.26 (d, *J* = 7.8 Hz, 2H), 1.60 (s, 3H), 1.55 (s, 3H), 1.19 (d, *J* = 6.9 Hz, 24H), 1.09 (d, *J* = 6.9 Hz, 24H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.53 (2xC, C carbene), 169.38 (2xC, <u>CO</u>OMe), 145.61 (8xC, CqAr*i*Pr), 136.79 (Cq enyne), 133.71 (4xC, CqArN), 130.92 (4xC, CHArpara), 124.33 (8xC, CHArmeta), 124.29 (4xC, CH imidazole), 120.88, 116.92 (CH enyne), 107.64, 57.75 (Cq enyne), 52.61 (2xC, COO<u>CH$_3$</u>), 30.25 (CH_2 enyne), 28.80 (8xC), 26.13 (CH_3 enyne), 25.64 (8xC), 24.71 (CH_2 enyne), 23.94 (8xC), 17.97 (CH_3 enyne).

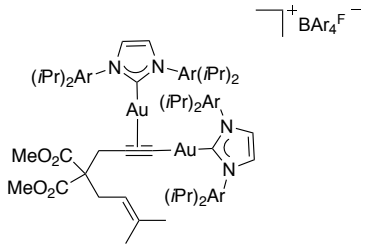
IR (neat) 3170, 2962, 2928, 2870, 1739, 1459, 1385, 1365, 1224, 1178, 804, 756, 655 cm^{-1}.

HRMS-ESI: calculated for $C_{67}H_{89}Au_2N_4O_4$ $[M-SbF_6]^+$: 1407.6210; found = 1407.6199.

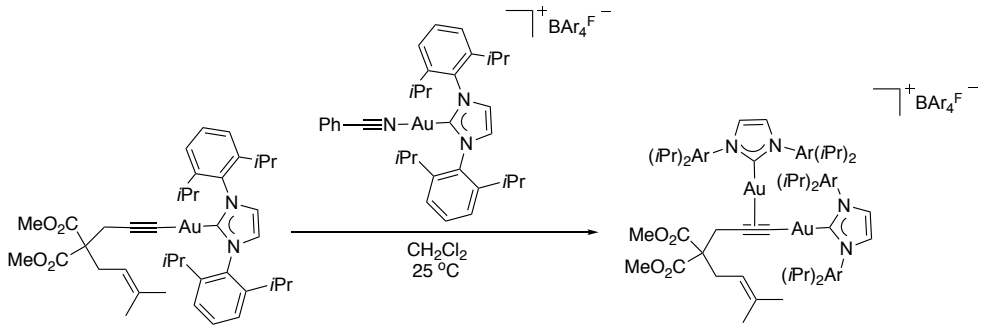
Melting point: 174-184 °C decomposition.

Structure confirmed by X-ray crystallography: CCDC 1572066.

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl] borate (14b)



The title compound was prepared according to the procedure below, and obtained as a beige solid (26.3 mg, 0.012 mmol, 95%).



To a solution of [(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)]gold (10 mg, 0.012 mmol, 1 equiv) in CH_2Cl_2 (1.2 mL) was added benzonitrile[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (18.86 mg, 0.012 mmol, 1 equiv) solid and the mixture was stirred for 1 h. The crude was concentrated, de resulting oil diluted in CH_2Cl_2, then filtered through Celite, through Teflon 0.22 and concentrated to afford a solid that was washed with pentane.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76-7.68 (m, 8H), 7.54 (s, 4H), 7.51 (t, *J* = 7.8 Hz, 4H), 7.26 (d, *J* = 8.2 Hz, 8H), 7.17 (s, 4H), 4.55 (t, *J* = 7.4 Hz, 1H), 3.46 (s, 6H), 2.41 (hept, *J* = 7.1 Hz, 8H), 2.27 (d, *J* = 3.3 Hz, 2H), 2.28 (s, 2H), 1.61 (s, 3H), 1.53 (s, 3H), 1.18 (d, *J* = 6.9 Hz, 24H), 1.10 (d, *J* = 6.9 Hz, 24H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.00 (2xC, C carbene), 169.33 (2xC, <u>CO</u>OMe), 161.84 (q, *J* (^{13}C-^{11}B) = 50.72 Hz, (4xC, Cq)) 145.55 (8xC, CqAr*i*Pr), 136.88 (Cq enyne), 134.96 (8xC, CHArorto BAr_4F), 133.56 (4xC, CqArN), 131.08 (4xC, CHArpara), 128.90 (qdd, *J* (^{13}C-^{19}F) = 31.0, 5.4, 2.8 Hz (8xC, Cq)), 124.72 (q, *J* (^{13}C-^{19}F) = 272.5 Hz (8xC, Cq)), 124.42 (8xC, CHArmeta), 123.93 (4xC, CH imidazole), 120.65 (overlapped with q, Cq BAr_4F), 117.57 (dt, *J* (^{13}C-^{19}F) = 7.0, 3.2 Hz (4xC, CHArpara BAr_4F))116.85 (CH enyne), 108.04, 57.73 (Cq enyne), 52.61 (2xC, COO<u>CH_3</u>), 30.24 (CH_2 enyne), 28.86 (8xC), 26.11 (CH_3 enyne), 25.63 (CH_2 enyne) 24.67 (8xC), 23.87 (8xC), 17.96 (CH_3 enyne).

^{19}F{^{1}H} NMR (376 MHz, $CDCl_3$) δ -62.16.

^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$) δ -6.68.

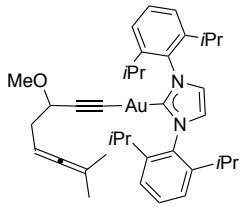
IR (neat) 2966, 2929, 1731, 1469, 1354, 1277, 1121, 886, 803, 757, 681 cm^{-1}.

HRMS-ESI: calculated for $C_{67}H_{89}Au_2N_4O_4$ $[M-C_{32}H_{12}BF_{24}]^+$: 1407.6210; found = 1407.6230.

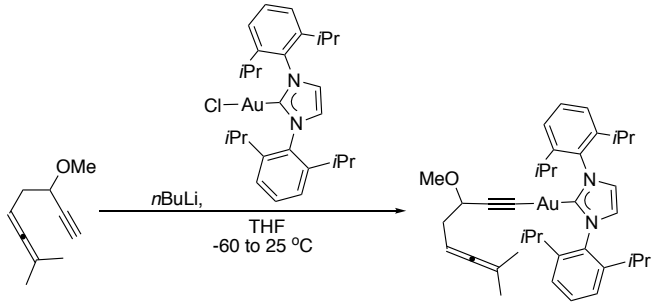
Melting point: 112-133 °C decomposition.

Structure confirmed by X-ray crystallography: CCDC 1572071.

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(3-methoxy-7-methylocta-5,6-dien-1-yne)]gold (19)



The title compound was prepared according to the procedure below, and obtained as a beige solid (50.0 mg, 0.057 mmol, 85%).



An oven-dried schlenk or vial under argon atmosphere was charged with 3-methoxy-7-methylocta-5,6-dien-1-yne (18.14 mg, 0.121 mmol, 1.5 equiv) in anhydrous THF (0.8 mL) the resulting solution was cooled to -60 ºC before adding *n*BuLi (2.5 M in hexanes, 0.058 mL, 0.145 mmol, 1.8 equiv) dissolved in 0.2 mL anhydrous THF and stirring for 30 min at this temperature. Chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (50 mg, 0.081 mmol, 1 equiv) was dissolved in anhydrous THF (2.2 mL) under Ar and added to the reaction mixture. The cooling bath was maintained for 15 min and then the mixture was stirred at 25 ºC for 10 h. The crude was concentrated, dissolved in CH_2Cl_2 and filtered through cotton and Teflon 0.22. The solvent was removed and the resulting solid was washed with pentane.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (t, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 4H), 7.10 (s, 2H), 5.00-4.88 (m, 1H), 4.00 (t, *J* = 6.3 Hz, 1H), 3.28 (s, 3H), 2.58 (hept, *J* = 7.5 Hz, 4H), 2.23 (t, *J* = 6.6 Hz, 2H), 1.58 (dd, *J* = 4.3, 2.9 Hz, 6H), 1.34 (d, *J* = 6.8 Hz, 12H), 1.20 (d, *J* = 6.9 Hz, 12H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 202.75 (Cq allene), 191.50 (C carbene), 145.75 (4xC, CqAr*i*Pr), 134.50 (2xC, CqArN), 130.54 (2xC, CHArpara), 124.28 (4xC, CHArmeta), 123.68 (Cq alkene), 123.23 (2xC, CH imidazole), 101.14, 94.51, 85.27 (CH allene), 72.00 ($\underline{CH}OCH_3$), 55.78 ($CHO\underline{CH_3}$), 37.05 (CH_2 allene), 28.94 (4xC), 24.63 (4xC), 24.18 (4xC), 20.82 (CH_3 enyne), 20.79 (CH_3 allene).

IR (neat) 3074, 2961, 2867, 2813, 1465, 1415, 1329, 1081, 803, 759 cm^{-1}.

HRMS-ESI: calculated for $C_{37}H_{50}AuN_2O$ $[M+H]^+$: 735.3583; found = 735.3604. Anal. calcd. For $C_{37}H_{49}AuN_2O$: C, 60.48; H, 6.72; N, 3.81; found: C, 60.21; H, 6.50; N, 3.94.

Melting point: 157-159 °C.

3. High temperature NMR experiments

Figure S1. ^{1}H NMR (500 MHz) spectrum of complex **16** in 1,1,2,2-tetrachloroethane from 25 to 130 °C.

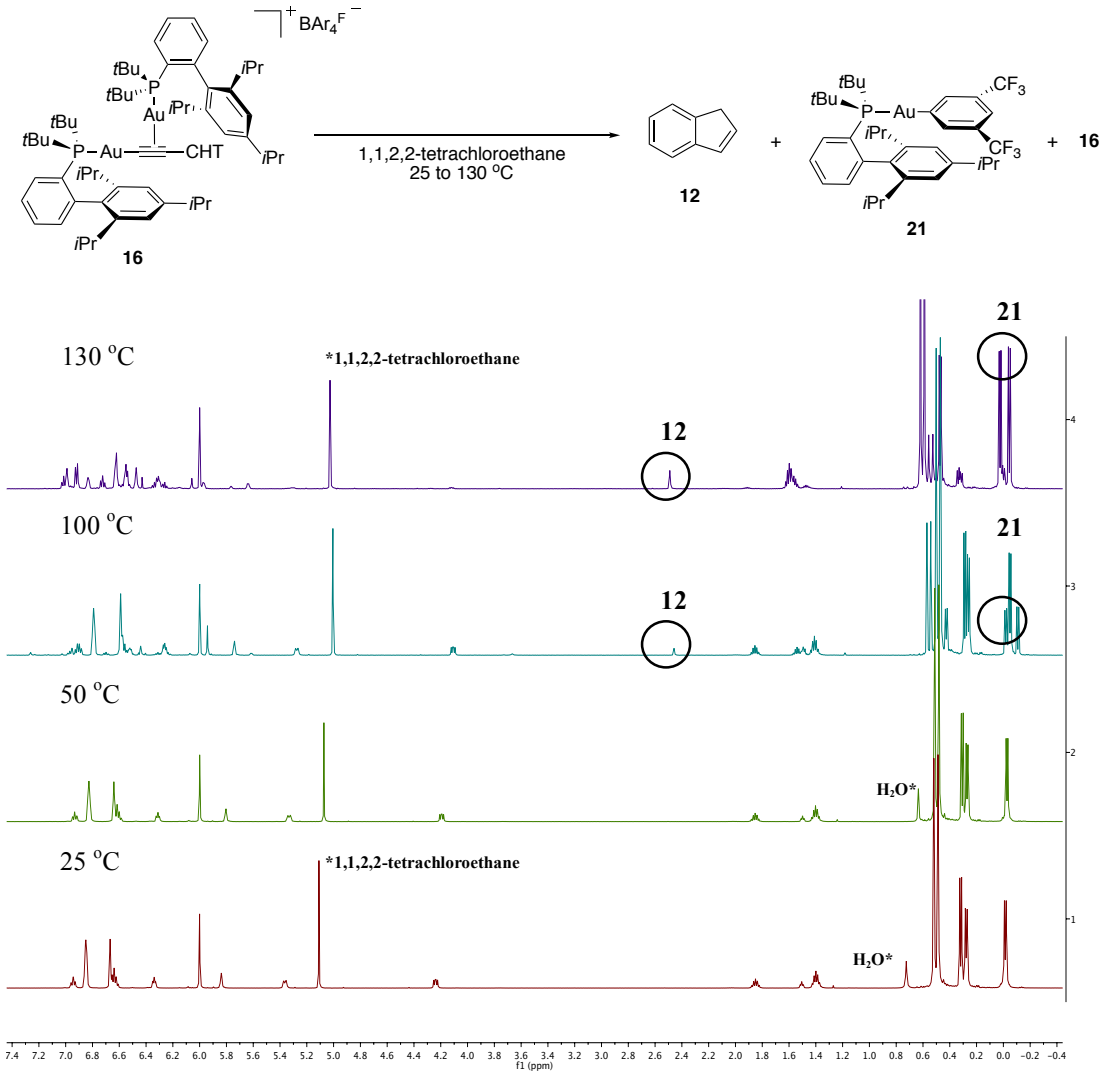


Figure S2. ^{31}P NMR (202 MHz) spectrum of complex **16** in 1,1,2,2-tetrachloroethane from 25 to 130 ^{o}C.

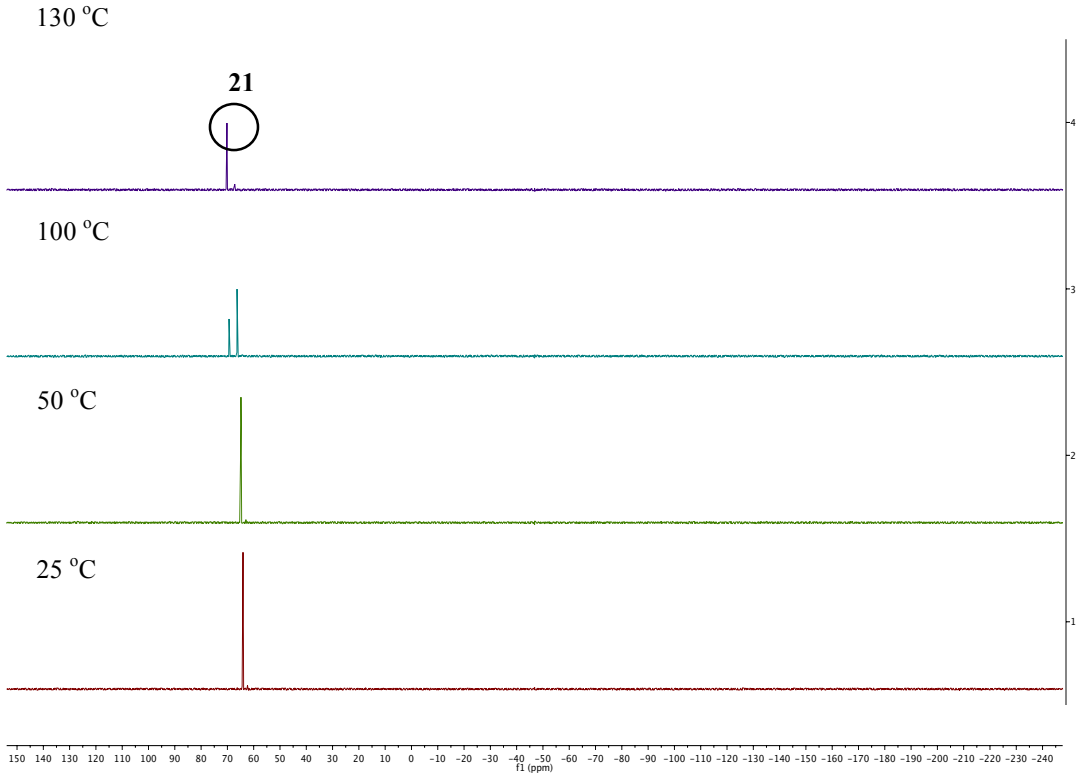


Figure S3. ^{1}H NMR (500 MHz) spectrum of complex **18b** in 1,1,2,2-tetrachloroethane from 25 to 130 °C.

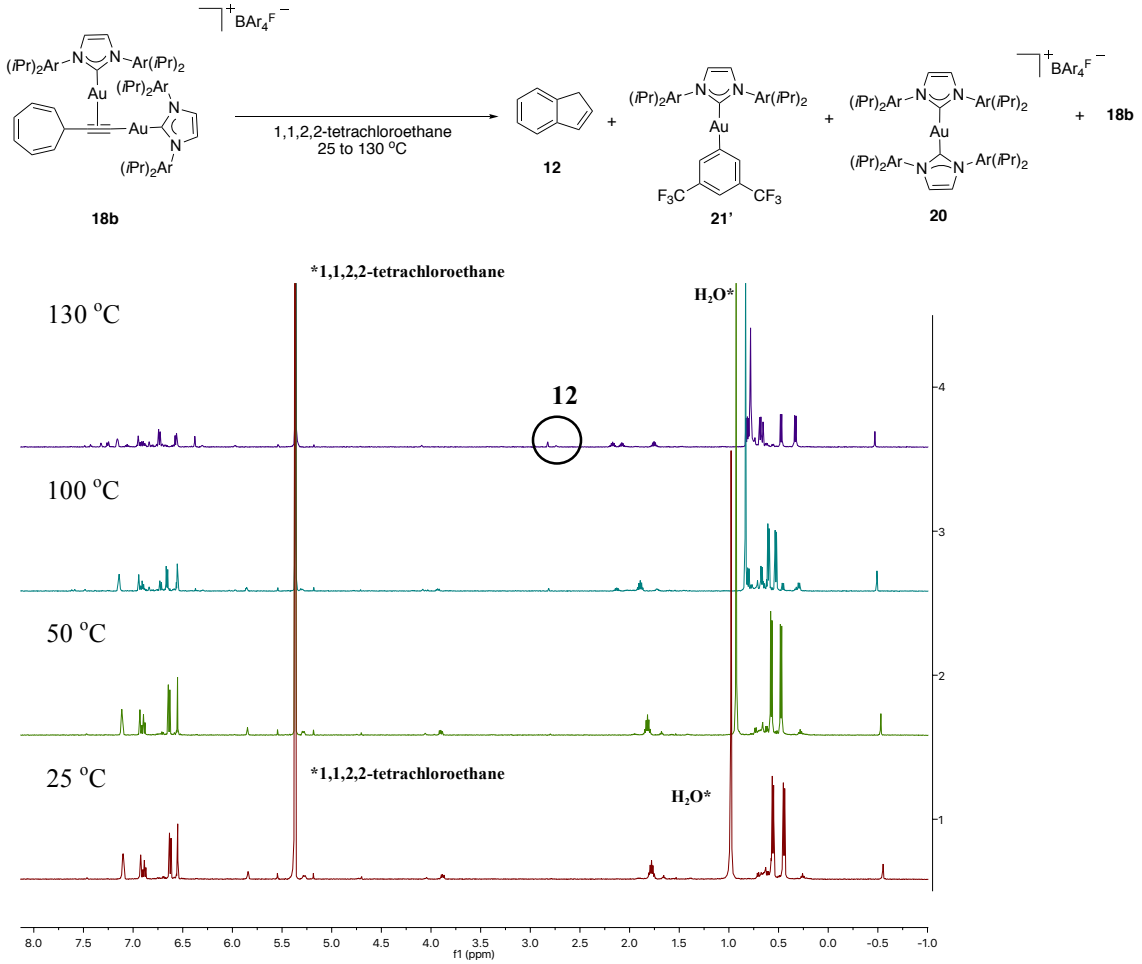


Figure S4. ^{19}F NMR (471 MHz) of complex **18b** in 1,1,2,2-tetrachloroethane from 25 to 130 °C.

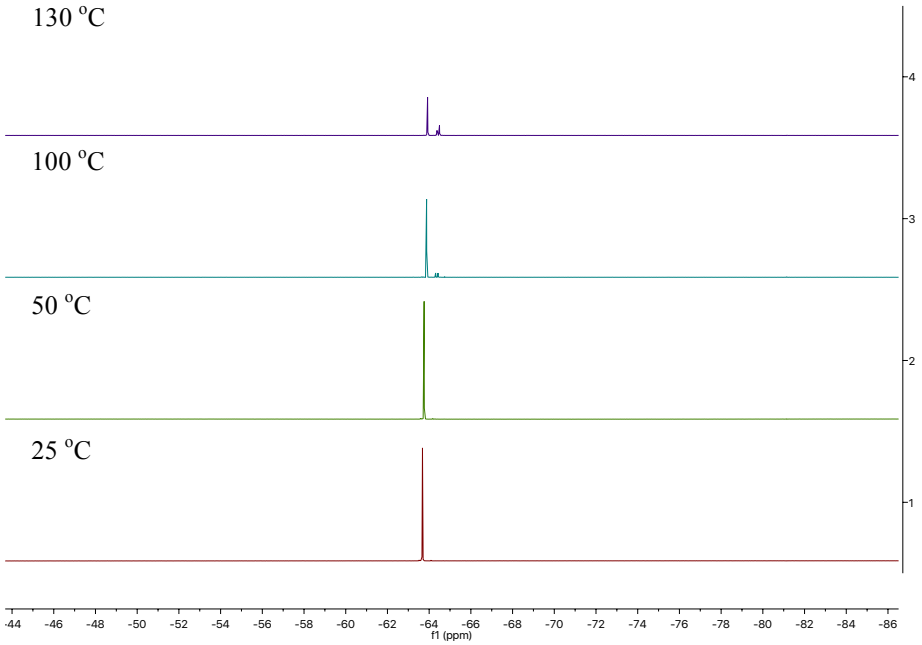


Figure S5. ^{1}H NMR (500 MHz) of complex **14b** in 1,1,2,2-tetrachloroethane from 25 to 130 °C.

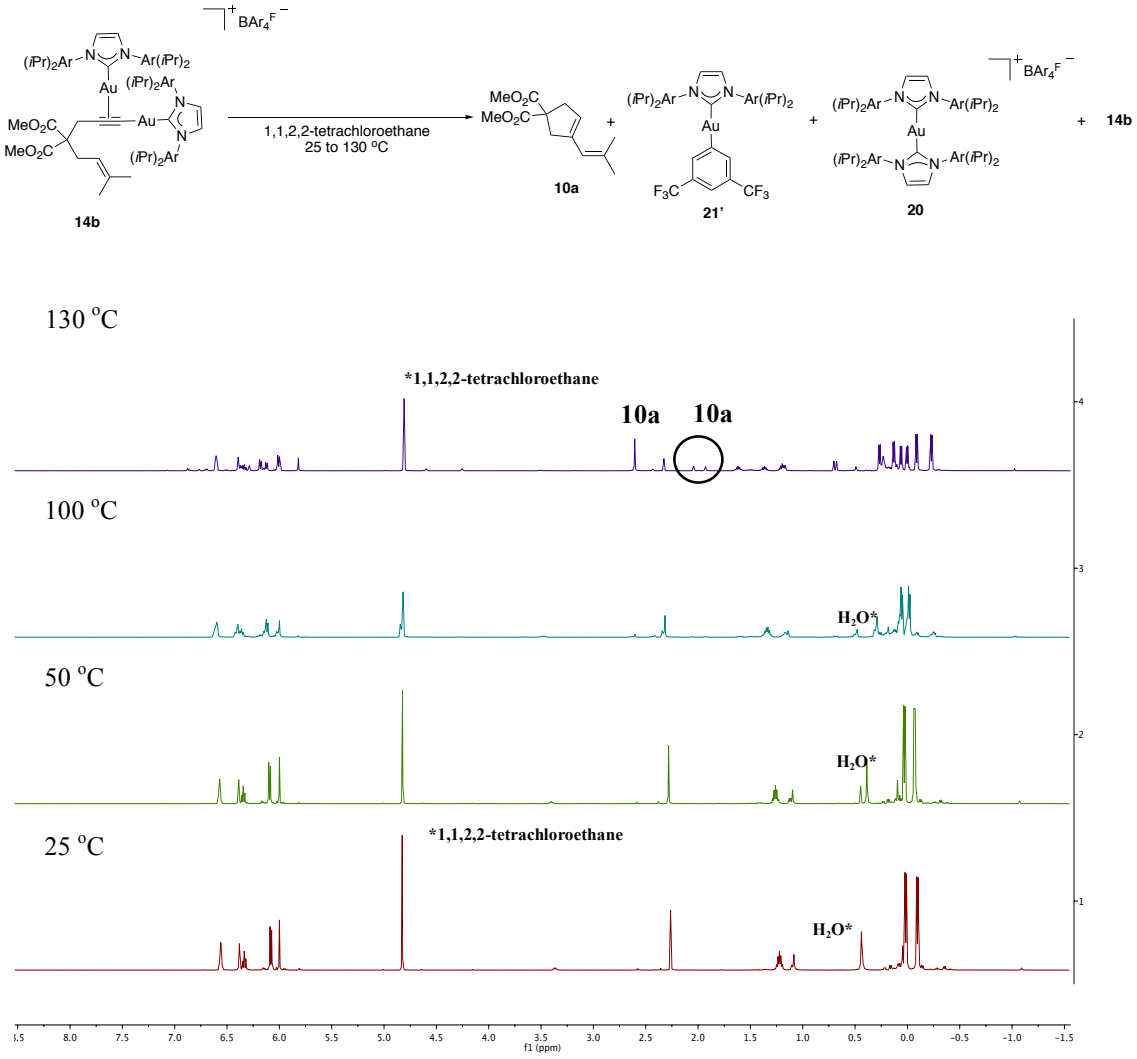


Figure S6. ^{1}H NMR (500 MHz) of complex **14a** in 1,1,2,2-tetrachloroethane from 25 to 130 ^{o}C.

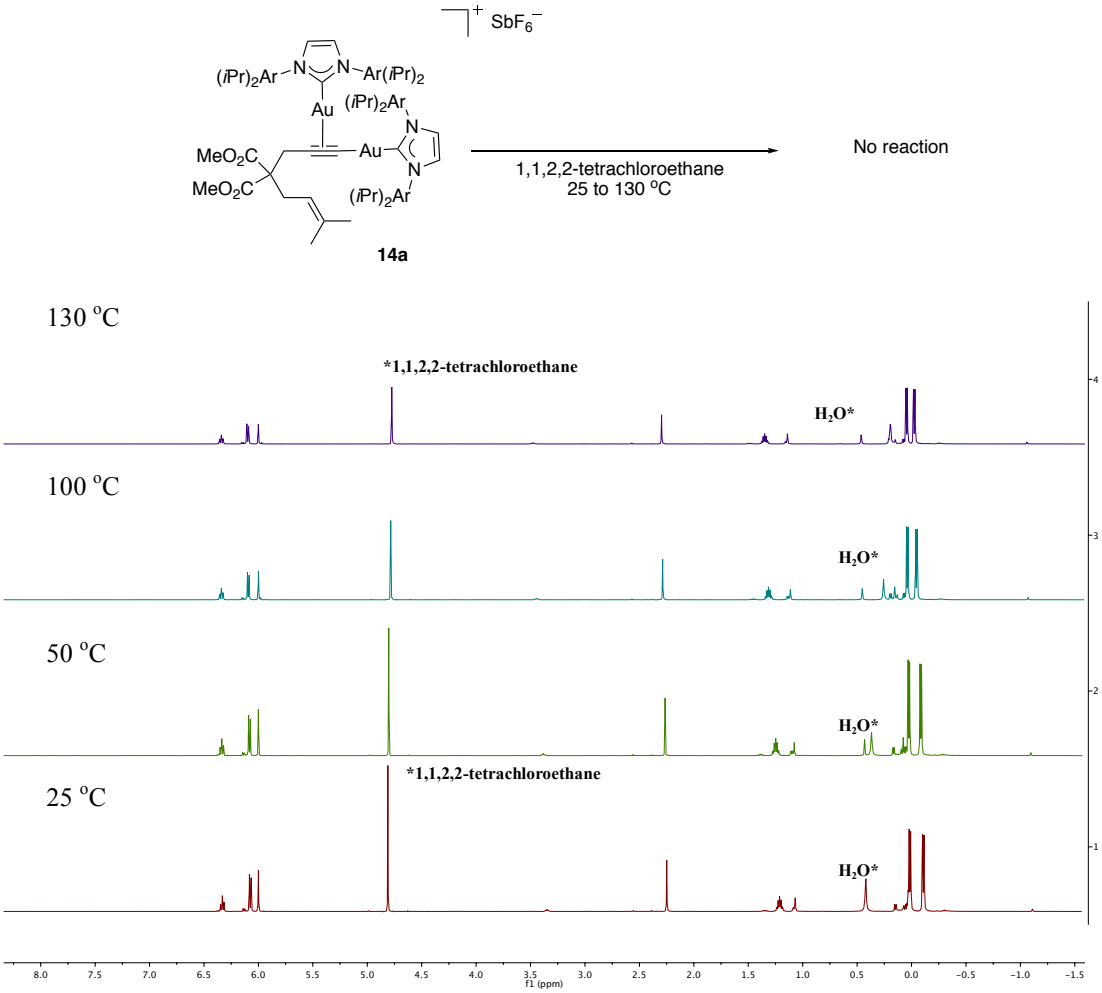
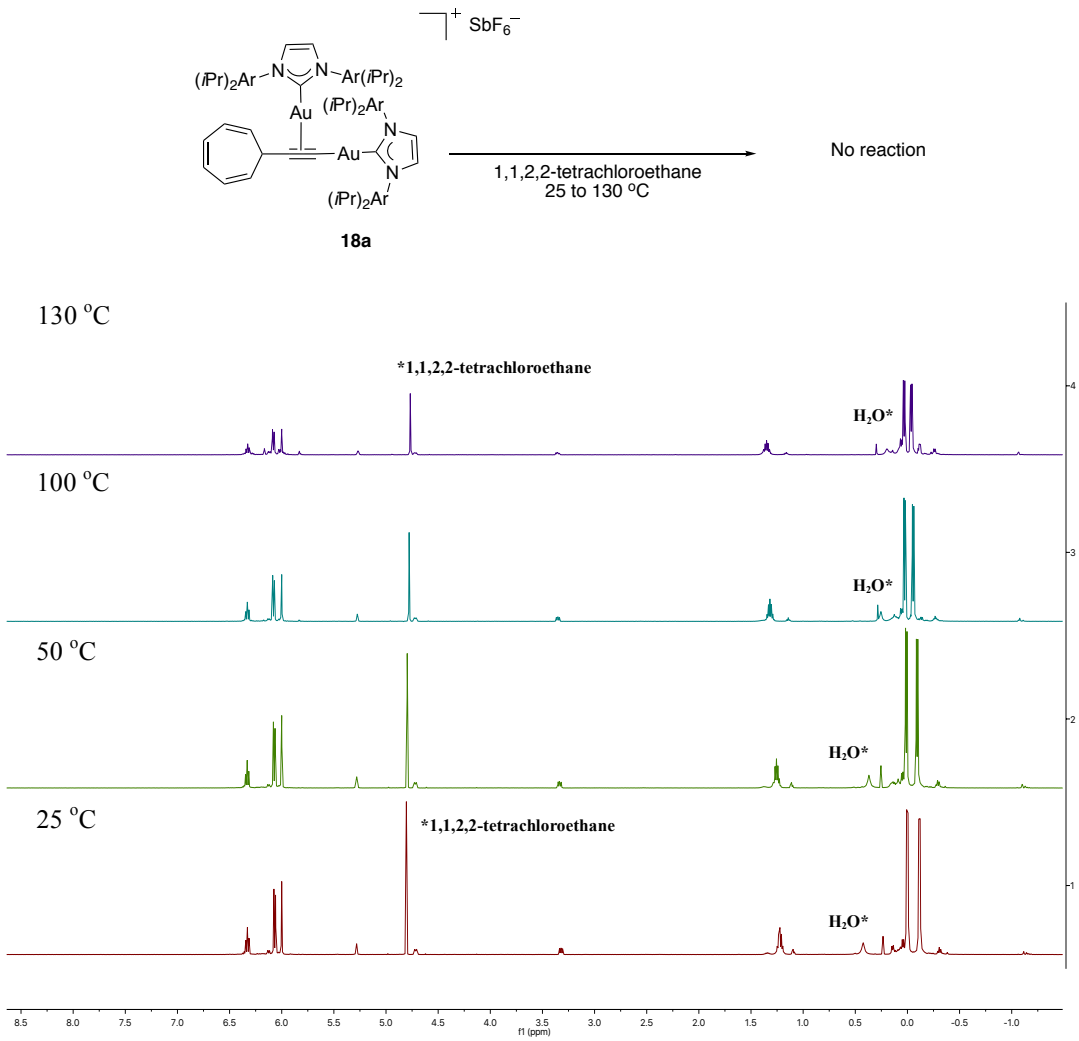


Figure S7. ^{1}H NMR (500 MHz) of complex **18a** in 1,1,2,2-tetrachloroethane from 25 to 130 °C.



4. Crystal Data and Structure Refinement

[(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine](2-cyclohepta-2,4,6-trien-1-ylethynyl)gold (15) CCDC 1572067.

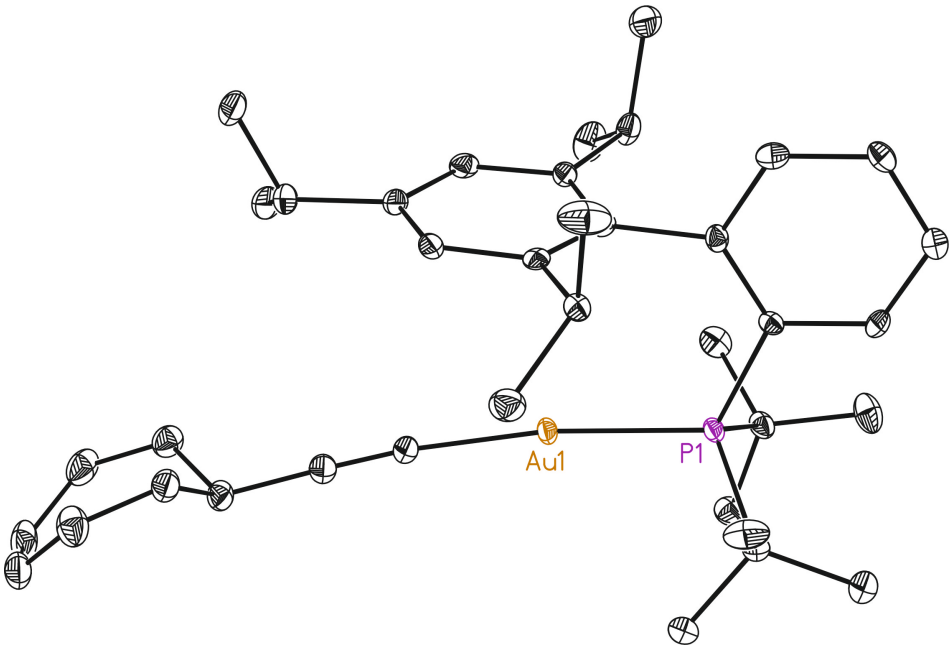


Table 1. Crystal data and structure refinement for mo_SFCA8_0m.

Identification code	mo_SFCA8_0m	
Empirical formula	C38 H52 Au P	
Formula weight	736.73	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.6685(5)Å	a= 90°.
	b = 13.5518(6)Å	b = 90°.
	c = 23.7502(11)Å	g = 90°.
Volume	3433.7(3) $Å^3$	
Z	4	
Density (calculated)	1.425 Mg/m^3	
Absorption coefficient	4.354 mm^{-1}	
F(000)	1496	
Crystal size	0.40 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.730 to 30.553°.	
Index ranges	-15<=h<=14,-12<=k<=18,-33<=l<=28	
Reflections collected	33739	

Independent reflections	10112[R(int) = 0.0375]
Completeness to theta =30.553°	97.1%
Absorption correction	Multi-scan
Max. and min. transmission	0.476 and 0.309
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10112/ 0/ 373
Goodness-of-fit on F^2	0.989
Final R indices [I>2sigma(I)]	R1 = 0.0247, wR2 = 0.0463
R indices (all data)	R1 = 0.0286, wR2 = 0.0473
Flack parameter	x =-0.011(3)
Largest diff. peak and hole	0.756 and -0.642 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for mo_SFCA8_0m.

Bond lengths----	
Au1-C1	2.007(4)
Au1-P1	2.2961(9)
C1-C2	1.200(5)
C2-C3	1.481(5)
C3-C4	1.500(5)
C3-C9	1.505(5)
C4-C5	1.344(6)
C5-C6	1.437(7)
C6-C7	1.339(6)
C7-C8	1.436(6)
C8-C9	1.345(6)
C10-C11	1.403(5)
C10-C15	1.406(5)
C10-P1	1.843(4)
C11-C12	1.377(5)
C12-C13	1.376(6)
C13-C14	1.389(6)
C14-C15	1.400(5)
C15-C16	1.515(5)
C16-C21	1.403(5)
C16-C17	1.413(5)
C17-C18	1.403(5)
C17-C22	1.517(5)
C18-C19	1.388(5)

C19-C20	1.389(5)
C19-C25	1.519(5)
C20-C21	1.392(5)
C21-C28	1.526(5)
C22-C24	1.530(6)
C22-C23	1.534(6)
C25-C27	1.523(6)
C25-C26	1.528(5)
C28-C29	1.526(5)
C28-C30	1.530(5)
C31-C34	1.535(5)
C31-C33	1.535(6)
C31-C32	1.539(5)
C31-P1	1.893(4)
C35-C37	1.529(5)
C35-C38	1.535(6)
C35-C36	1.539(5)
C35-P1	1.888(4)

Angles----------

C1-Au1-P1	172.86(11)
C2-C1-Au1	173.7(4)
C1-C2-C3	174.0(5)
C2-C3-C4	115.1(3)
C2-C3-C9	111.3(3)
C4-C3-C9	107.6(3)
C5-C4-C3	121.4(4)
C4-C5-C6	125.4(4)
C7-C6-C5	126.2(4)
C6-C7-C8	125.3(4)
C9-C8-C7	125.2(4)
C8-C9-C3	121.5(4)
C11-C10-C15	117.9(3)
C11-C10-P1	117.8(3)
C15-C10-P1	124.3(3)
C12-C11-C10	123.4(4)
C13-C12-C11	118.5(4)
C12-C13-C14	119.6(4)

C13-C14-C15	122.5(4)
C14-C15-C10	118.1(3)
C14-C15-C16	115.7(3)
C10-C15-C16	126.3(3)
C21-C16-C17	119.9(3)
C21-C16-C15	119.7(3)
C17-C16-C15	120.2(3)
C18-C17-C16	118.5(3)
C18-C17-C22	118.9(3)
C16-C17-C22	122.6(3)
C19-C18-C17	122.4(3)
C18-C19-C20	117.4(3)
C18-C19-C25	122.9(3)
C20-C19-C25	119.7(3)
C19-C20-C21	122.8(4)
C20-C21-C16	118.8(4)
C20-C21-C28	119.4(3)
C16-C21-C28	121.7(3)
C17-C22-C24	113.0(3)
C17-C22-C23	111.0(3)
C24-C22-C23	109.8(4)
C19-C25-C27	113.3(3)
C19-C25-C26	111.5(3)
C27-C25-C26	111.1(3)
C21-C28-C29	109.9(3)
C21-C28-C30	112.3(3)
C29-C28-C30	111.0(3)
C34-C31-C33	107.0(3)
C34-C31-C32	107.6(3)
C33-C31-C32	108.5(3)
C34-C31-P1	108.0(3)
C33-C31-P1	117.8(3)
C32-C31-P1	107.6(3)
C37-C35-C38	108.9(3)
C37-C35-C36	109.8(3)
C38-C35-C36	107.1(3)
C37-C35-P1	107.9(3)
C38-C35-P1	105.8(3)

C36-C35-P1	116.9(3)
C10-P1-C35	105.46(17)
C10-P1-C31	106.97(16)
C35-P1-C31	111.51(17)
C10-P1-Au1	116.09(12)
C35-P1-Au1	109.24(13)
C31-P1-Au1	107.60(13)

Table 3. Torsion angles [°] for mo_SFCA8_0m.

C2-C3-C4-C5	169.4(4)
C9-C3-C4-C5	-65.8(5)
C3-C4-C5-C6	6.4(7)
C4-C5-C6-C7	32.2(8)
C5-C6-C7-C8	1.4(8)
C6-C7-C8-C9	-33.3(8)
C7-C8-C9-C3	-7.5(7)
C2-C3-C9-C8	-165.9(4)
C4-C3-C9-C8	67.1(5)
C15-C10-C11-C12	-0.9(6)
P1-C10-C11-C12	179.7(3)
C10-C11-C12-C13	0.5(6)
C11-C12-C13-C14	0.4(6)
C12-C13-C14-C15	-0.9(6)
C13-C14-C15-C10	0.5(6)
C13-C14-C15-C16	179.0(4)
C11-C10-C15-C14	0.4(5)
P1-C10-C15-C14	179.8(3)
C11-C10-C15-C16	-178.0(3)
P1-C10-C15-C16	1.4(5)
C14-C15-C16-C21	-90.5(4)
C10-C15-C16-C21	87.9(5)
C14-C15-C16-C17	84.7(4)
C10-C15-C16-C17	-97.0(5)
C21-C16-C17-C18	-5.9(5)
C15-C16-C17-C18	178.9(3)
C21-C16-C17-C22	171.6(3)
C15-C16-C17-C22	-3.6(6)

C16-C17-C18-C19	1.3(6)
C22-C17-C18-C19	-176.3(4)
C17-C18-C19-C20	3.6(6)
C17-C18-C19-C25	-175.7(3)
C18-C19-C20-C21	-4.2(5)
C25-C19-C20-C21	175.2(3)
C19-C20-C21-C16	-0.3(5)
C19-C20-C21-C28	176.6(3)
C17-C16-C21-C20	5.4(5)
C15-C16-C21-C20	-179.4(3)
C17-C16-C21-C28	-171.4(3)
C15-C16-C21-C28	3.8(5)
C18-C17-C22-C24	-40.4(5)
C16-C17-C22-C24	142.2(4)
C18-C17-C22-C23	83.5(4)
C16-C17-C22-C23	-94.0(4)
C18-C19-C25-C27	29.4(5)
C20-C19-C25-C27	-149.9(4)
C18-C19-C25-C26	-96.9(4)
C20-C19-C25-C26	83.8(4)
C20-C21-C28-C29	-82.3(4)
C16-C21-C28-C29	94.5(4)
C20-C21-C28-C30	41.8(5)
C16-C21-C28-C30	-141.5(4)
C11-C10-P1-C35	-65.3(3)
C15-C10-P1-C35	115.3(3)
C11-C10-P1-C31	53.5(3)
C15-C10-P1-C31	-125.8(3)
C11-C10-P1-Au1	173.6(2)
C15-C10-P1-Au1	-5.7(3)
C37-C35-P1-C10	172.5(3)
C38-C35-P1-C10	-70.9(3)
C36-C35-P1-C10	48.2(3)
C37-C35-P1-C31	56.8(3)
C38-C35-P1-C31	173.3(3)
C36-C35-P1-C31	-67.6(3)
C37-C35-P1-Au1	-62.0(3)
C38-C35-P1-Au1	54.5(3)

C36-C35-P1-Au1	173.6(3)
C34-C31-P1-C10	160.7(3)
C33-C31-P1-C10	-78.1(3)
C32-C31-P1-C10	44.8(3)
C34-C31-P1-C35	-84.5(3)
C33-C31-P1-C35	36.8(3)
C32-C31-P1-C35	159.7(3)
C34-C31-P1-Au1	35.3(3)
C33-C31-P1-Au1	156.5(3)
C32-C31-P1-Au1	-80.6(3)

{[(2´,4´,6´-Triisopropyl-1,1´-biphenyl-2-yl)di-*tert*-butylphosphine](2-cyclohepta-2,4,6-trien-1-ylethynyl)gold}[(2´,4´,6´-Triisopropyl-1,1´-biphenyl-2-yl)di-*tert*-butylphosphine] gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (16) CCDC 1572069.

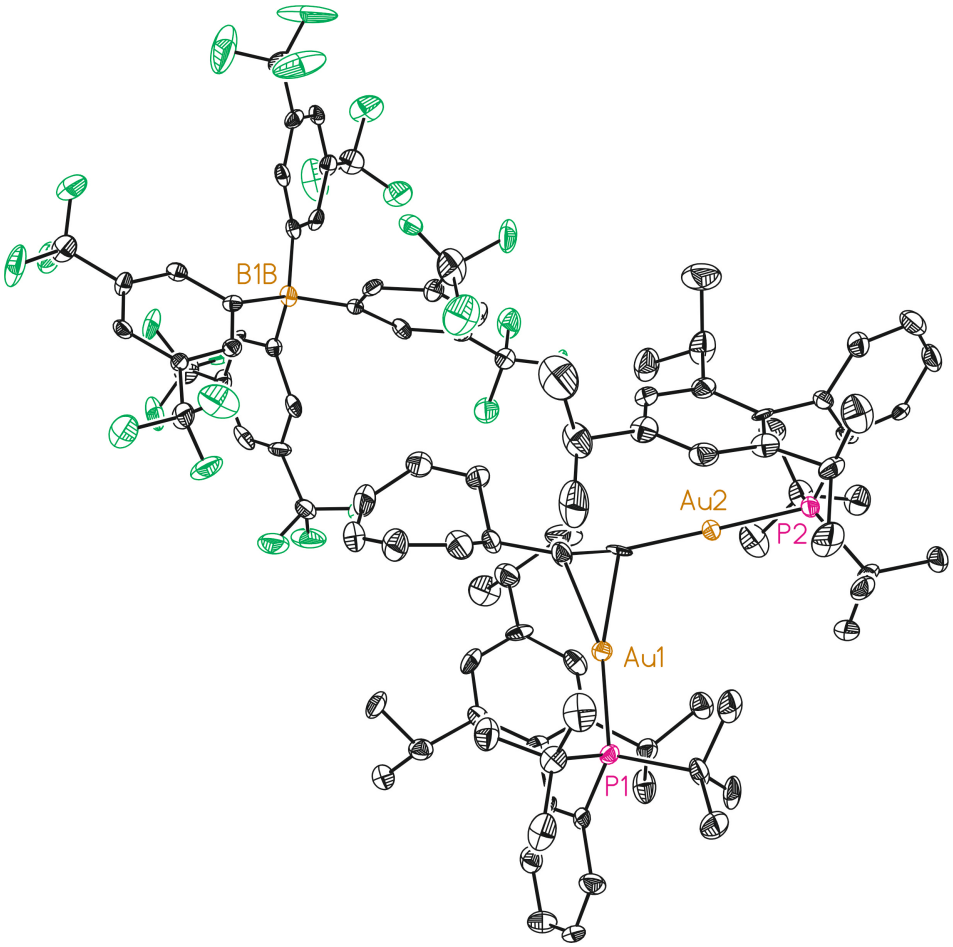


Table 1. Crystal data and structure refinement for mo_SFCA9.

Identification code	mo_SFCA9	
Empirical formula	C99 H109 Au2 B F24 P2	
Formula weight	2221.54	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 47.359(3)Å	a= 90°.
	b = 12.9120(8)Å	b = 90°.
	c = 16.1240(7)Å	g = 90°.
Volume	9859.8(9) $Å^3$	
Z	4	
Density (calculated)	1.497 Mg/m^3	
Absorption coefficient	3.094 mm^{-1}	
F(000)	4448	
Crystal size	0.20 x 0.10 x 0.02 mm^3	
Theta range for data collection	1.796 to 27.120°.	
Index ranges	-34<=h<=60,-9<=k<=16,-20<=l<=13	
Reflections collected	48513	
Independent reflections	19433[R(int) = 0.0778]	
Completeness to theta =27.120°	99.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.941 and 0.724	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19433/ 158/ 1288	
Goodness-of-fit on F^2	0.915	
Final R indices [I>2sigma(I)]	R1 = 0.0482, wR2 = 0.0877	
R indices (all data)	R1 = 0.0875, wR2 = 0.1016	
Flack parameter	x =0.005(4)	
Largest diff. peak and hole	1.407 and -1.404 e.$Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for mo_SFCA9.

Bond lengths----	
Au1-C1	2.224(10)
Au1-C2	2.253(11)
Au1-P1	2.287(3)

Au2-C1	2.026(12)
Au2-P2	2.297(3)
C1-C2	1.214(15)
C2-C3	1.506(16)
C3-C4	1.487(17)
C3-C9	1.510(17)
C4-C5	1.320(18)
C5-C6	1.409(18)
C6-C7	1.343(19)
C7-C8	1.41(2)
C8-C9	1.348(19)
C10-C11	1.410(15)
C10-C15	1.420(15)
C10-P1	1.816(12)
C11-C12	1.356(17)
C12-C13	1.369(17)
C13-C14	1.389(17)
C14-C15	1.406(16)
C15-C16	1.502(15)
C16-C17	1.394(15)
C16-C21	1.403(16)
C17-C18	1.409(15)
C17-C22	1.513(15)
C18-C19	1.413(15)
C19-C20	1.396(16)
C19-C25	1.498(16)
C20-C21	1.390(16)
C21-C28	1.528(15)
C22-C24	1.538(15)
C22-C23	1.559(16)
C25-C27	1.541(16)
C25-C26	1.550(18)
C28-C30	1.527(16)
C28-C29	1.532(16)
C31-C34	1.513(15)
C31-C32	1.537(16)
C31-C33	1.546(16)
C31-P1	1.866(12)

C35-C37	1.492(16)
C35-C36	1.522(18)
C35-C38	1.542(18)
C35-P1	1.906(12)
C39-C40	1.396(14)
C39-C44	1.435(15)
C39-P2	1.842(11)
C40-C41	1.358(15)
C41-C42	1.361(16)
C42-C43	1.398(17)
C43-C44	1.394(16)
C44-C45	1.492(16)
C45-C46	1.389(15)
C45-C50	1.423(16)
C46-C47	1.415(17)
C46-C51	1.530(16)
C47-C48	1.386(17)
C48-C49	1.369(17)
C48-C54	1.522(17)
C49-C50	1.394(17)
C50-C57	1.524(16)
C51-C53	1.553(16)
C51-C52	1.561(17)
C54-C56	1.484(19)
C54-C55	1.504(19)
C57-C58	1.522(19)
C57-C59	1.529(17)
C60-C63	1.522(17)
C60-C61	1.527(16)
C60-C62	1.529(16)
C60-P2	1.906(11)
C64-C67	1.523(17)
C64-C65	1.544(17)
C64-C66	1.544(18)
C64-P2	1.909(12)
B1B-C1B	1.622(15)
B1B-C9B	1.632(15)
B1B-C25B	1.633(16)

B1B-C17B	1.637(16)
C1B-C2B	1.404(15)
C1B-C6B	1.421(14)
C2B-C3B	1.381(15)
C3B-C4B	1.377(16)
C3B-C7B	1.535(17)
C4B-C5B	1.395(16)
C5B-C6B	1.381(15)
C5B-C8B	1.515(15)
C7B-F3B	1.317(14)
C7B-F2B	1.327(14)
C7B-F1B	1.350(14)
C8B-F4B	1.328(12)
C8B-F6B"	1.329(12)
C8B-F6B	1.331(12)
C8B-F6B'	1.336(12)
C8B-F4B'	1.338(12)
C8B-F5B"	1.338(11)
C8B-F5B'	1.349(12)
C8B-F5B	1.359(12)
C8B-F4B"	1.372(11)
C9B-C10B	1.384(14)
C9B-C14B	1.405(15)
C10B-C11B	1.384(14)
C11B-C12B	1.403(14)
C11B-C15B	1.507(15)
C12B-C13B	1.361(15)
C13B-C14B	1.402(16)
C13B-C16B	1.519(16)
C15B-F7B	1.312(14)
C15B-F8B	1.328(13)
C15B-F9B	1.354(13)
C16B-F10B	1.322(14)
C16B-F12B	1.328(15)
C16B-F11B	1.330(15)
C17B-C22B	1.389(15)
C17B-C18B	1.416(15)
C18B-C19B	1.380(16)

C19B-C20B	1.369(15)
C19B-C23B	1.490(16)
C20B-C21B	1.381(16)
C21B-C22B	1.383(15)
C21B-C24B	1.514(15)
C23B-F13B	1.284(13)
C23B-F14B	1.290(15)
C23B-F15B	1.313(15)
C24B-F16B	1.325(14)
C24B-F18B	1.330(14)
C24B-F17B	1.329(14)
C25B-C26B	1.387(14)
C25B-C30B	1.400(15)
C26B-C27B	1.397(15)
C27B-C28B	1.388(16)
C27B-C31B	1.503(15)
C28B-C29B	1.381(17)
C29B-C30B	1.362(16)
C29B-C32B	1.499(17)
C31B-F20'	1.327(12)
C31B-F19B	1.330(12)
C31B-F19'	1.341(12)
C31B-F21"	1.343(13)
C31B-F21B	1.348(12)
C31B-F21'	1.352(12)
C31B-F19"	1.347(13)
C31B-F20"	1.367(13)
C31B-F20B	1.358(12)
C32B-F22B	1.334(14)
C32B-F24B	1.337(15)
C32B-F23B	1.338(15)

Angles----------

C1-Au1-C2	31.5(4)
C1-Au1-P1	165.1(3)
C2-Au1-P1	160.0(3)
C1-Au2-P2	172.7(3)
C2-C1-Au2	169.7(10)

C2-C1-Au1	75.6(8)
Au2-C1-Au1	114.3(5)
C1-C2-C3	165.7(12)
C1-C2-Au1	73.0(7)
C3-C2-Au1	121.1(8)
C4-C3-C2	115.8(11)
C4-C3-C9	108.2(10)
C2-C3-C9	110.4(10)
C5-C4-C3	120.1(13)
C4-C5-C6	125.7(13)
C7-C6-C5	127.4(14)
C6-C7-C8	123.8(14)
C9-C8-C7	126.6(14)
C8-C9-C3	119.2(13)
C11-C10-C15	117.3(10)
C11-C10-P1	118.1(9)
C15-C10-P1	124.6(8)
C12-C11-C10	122.6(12)
C11-C12-C13	121.1(11)
C12-C13-C14	118.4(12)
C13-C14-C15	122.5(12)
C14-C15-C10	118.1(10)
C14-C15-C16	115.4(10)
C10-C15-C16	126.3(10)
C17-C16-C21	119.5(10)
C17-C16-C15	122.1(10)
C21-C16-C15	118.1(9)
C16-C17-C18	118.9(11)
C16-C17-C22	122.4(10)
C18-C17-C22	118.3(10)
C17-C18-C19	122.6(11)
C20-C19-C18	116.2(10)
C20-C19-C25	124.5(11)
C18-C19-C25	119.3(11)
C21-C20-C19	122.5(12)
C20-C21-C16	120.1(10)
C20-C21-C28	118.4(11)
C16-C21-C28	121.5(10)

C17-C22-C24	110.9(9)
C17-C22-C23	113.7(10)
C24-C22-C23	108.1(10)
C19-C25-C27	110.0(10)
C19-C25-C26	112.1(10)
C27-C25-C26	109.3(11)
C30-C28-C21	108.5(10)
C30-C28-C29	109.7(11)
C21-C28-C29	114.1(10)
C34-C31-C32	108.8(10)
C34-C31-C33	106.9(10)
C32-C31-C33	109.4(10)
C34-C31-P1	106.5(8)
C32-C31-P1	109.3(8)
C33-C31-P1	115.7(8)
C37-C35-C36	109.8(11)
C37-C35-C38	107.5(11)
C36-C35-C38	107.7(10)
C37-C35-P1	117.0(9)
C36-C35-P1	106.8(8)
C38-C35-P1	107.7(8)
C40-C39-C44	118.2(10)
C40-C39-P2	118.2(9)
C44-C39-P2	123.6(9)
C41-C40-C39	122.6(11)
C40-C41-C42	121.2(12)
C41-C42-C43	117.7(12)
C44-C43-C42	123.8(12)
C43-C44-C39	116.5(11)
C43-C44-C45	116.5(10)
C39-C44-C45	127.0(10)
C46-C45-C50	119.9(11)
C46-C45-C44	121.4(10)
C50-C45-C44	118.0(10)
C45-C46-C47	118.2(11)
C45-C46-C51	122.2(11)
C47-C46-C51	119.6(10)
C48-C47-C46	122.4(12)

C49-C48-C47	118.1(12)
C49-C48-C54	120.4(12)
C47-C48-C54	121.5(12)
C48-C49-C50	122.4(12)
C49-C50-C45	118.8(11)
C49-C50-C57	119.6(11)
C45-C50-C57	121.4(11)
C46-C51-C53	113.5(11)
C46-C51-C52	109.5(9)
C53-C51-C52	110.2(10)
C56-C54-C55	113.2(13)
C56-C54-C48	113.6(12)
C55-C54-C48	109.9(12)
C58-C57-C50	110.6(11)
C58-C57-C59	110.3(11)
C50-C57-C59	111.6(12)
C63-C60-C61	109.3(10)
C63-C60-C62	109.2(11)
C61-C60-C62	109.5(10)
C63-C60-P2	108.2(9)
C61-C60-P2	115.3(9)
C62-C60-P2	105.3(7)
C67-C64-C65	110.2(10)
C67-C64-C66	107.6(11)
C65-C64-C66	106.5(10)
C67-C64-P2	118.3(9)
C65-C64-P2	105.8(8)
C66-C64-P2	107.9(9)
C10-P1-C31	104.6(5)
C10-P1-C35	107.8(5)
C31-P1-C35	112.4(5)
C10-P1-Au1	116.9(4)
C31-P1-Au1	107.0(4)
C35-P1-Au1	108.3(4)
C39-P2-C60	105.4(5)
C39-P2-C64	107.4(5)
C60-P2-C64	111.5(5)
C39-P2-Au2	114.8(4)

C60-P2-Au2	110.4(4)
C64-P2-Au2	107.3(4)
C1B-B1B-C9B	113.4(8)
C1B-B1B-C25B	110.6(9)
C9B-B1B-C25B	102.6(9)
C1B-B1B-C17B	103.3(9)
C9B-B1B-C17B	113.8(9)
C25B-B1B-C17B	113.4(8)
C2B-C1B-C6B	115.7(10)
C2B-C1B-B1B	120.5(9)
C6B-C1B-B1B	123.3(9)
C3B-C2B-C1B	121.4(11)
C4B-C3B-C2B	122.3(11)
C4B-C3B-C7B	121.0(11)
C2B-C3B-C7B	116.8(10)
C3B-C4B-C5B	117.7(11)
C6B-C5B-C4B	120.8(11)
C6B-C5B-C8B	119.3(10)
C4B-C5B-C8B	120.0(10)
C5B-C6B-C1B	122.0(10)
F3B-C7B-F2B	108.8(10)
F3B-C7B-F1B	107.3(10)
F2B-C7B-F1B	105.8(10)
F3B-C7B-C3B	113.5(10)
F2B-C7B-C3B	110.9(10)
F1B-C7B-C3B	110.2(9)
F4B-C8B-F6B	109.0(13)
F6B'-C8B-F4B'	107.2(12)
F6B"-C8B-F5B"	108.2(12)
F6B'-C8B-F5B'	106.8(12)
F4B'-C8B-F5B'	107.0(12)
F4B-C8B-F5B	106.5(12)
F6B-C8B-F5B	107.2(12)
F6B"-C8B-F4B"	105.8(11)
F5B"-C8B-F4B"	104.5(11)
F4B-C8B-C5B	114.8(18)
F6B"-C8B-C5B	115.8(13)
F6B-C8B-C5B	112.6(19)

F6B'-C8B-C5B	109.7(14)
F4B'-C8B-C5B	116.1(15)
F5B"-C8B-C5B	112.5(13)
F5B'-C8B-C5B	109.6(15)
F5B-C8B-C5B	106.3(16)
F4B"-C8B-C5B	109.2(12)
C10B-C9B-C14B	114.7(10)
C10B-C9B-B1B	123.1(9)
C14B-C9B-B1B	121.6(9)
C9B-C10B-C11B	124.0(10)
C10B-C11B-C12B	120.1(10)
C10B-C11B-C15B	119.0(9)
C12B-C11B-C15B	120.9(10)
C13B-C12B-C11B	117.7(10)
C12B-C13B-C14B	121.5(10)
C12B-C13B-C16B	119.6(11)
C14B-C13B-C16B	118.8(10)
C13B-C14B-C9B	122.1(10)
F7B-C15B-F8B	107.4(10)
F7B-C15B-F9B	106.0(10)
F8B-C15B-F9B	105.7(9)
F7B-C15B-C11B	113.5(10)
F8B-C15B-C11B	112.5(10)
F9B-C15B-C11B	111.2(10)
F10B-C16B-F12B	107.0(12)
F10B-C16B-F11B	108.4(10)
F12B-C16B-F11B	106.4(10)
F10B-C16B-C13B	112.3(10)
F12B-C16B-C13B	111.4(10)
F11B-C16B-C13B	111.1(11)
C22B-C17B-C18B	114.1(10)
C22B-C17B-B1B	123.1(9)
C18B-C17B-B1B	122.1(9)
C19B-C18B-C17B	122.5(10)
C20B-C19B-C18B	120.5(10)
C20B-C19B-C23B	120.9(11)
C18B-C19B-C23B	118.6(10)
C19B-C20B-C21B	119.6(10)

C20B-C21B-C22B	119.0(11)
C20B-C21B-C24B	121.2(10)
C22B-C21B-C24B	119.8(11)
C21B-C22B-C17B	124.3(11)
F13B-C23B-F14B	105.4(12)
F13B-C23B-F15B	104.3(12)
F14B-C23B-F15B	105.2(11)
F13B-C23B-C19B	114.7(9)
F14B-C23B-C19B	113.0(11)
F15B-C23B-C19B	113.3(11)
F16B-C24B-F18B	106.4(10)
F16B-C24B-F17B	107.9(10)
F18B-C24B-F17B	106.2(10)
F16B-C24B-C21B	112.7(11)
F18B-C24B-C21B	111.1(9)
F17B-C24B-C21B	112.1(10)
C26B-C25B-C30B	114.3(10)
C26B-C25B-B1B	123.7(9)
C30B-C25B-B1B	121.7(10)
C25B-C26B-C27B	122.9(10)
C28B-C27B-C26B	120.2(11)
C28B-C27B-C31B	119.7(10)
C26B-C27B-C31B	120.1(10)
C29B-C28B-C27B	117.9(11)
C30B-C29B-C28B	120.7(11)
C30B-C29B-C32B	118.6(12)
C28B-C29B-C32B	120.7(11)
C29B-C30B-C25B	124.0(12)
F20'-C31B-F19'	108.7(11)
F19B-C31B-F21B	108.2(12)
F20'-C31B-F21'	108.0(12)
F19'-C31B-F21'	106.4(11)
F21"-C31B-F19"	106.9(13)
F21"-C31B-F20"	105.0(13)
F19"-C31B-F20"	104.9(13)
F19B-C31B-F20B	107.7(12)
F21B-C31B-F20B	105.2(11)
F20'-C31B-C27B	112.8(14)

F19B-C31B-C27B	115.1(14)
F19'-C31B-C27B	109.1(13)
F21"-C31B-C27B	114(2)
F21B-C31B-C27B	111.5(16)
F21'-C31B-C27B	111.6(14)
F19"-C31B-C27B	113(2)
F20"-C31B-C27B	112.0(16)
F20B-C31B-C27B	108.6(12)
F22B-C32B-F24B	105.8(10)
F22B-C32B-F23B	105.0(10)
F24B-C32B-F23B	106.9(12)
F22B-C32B-C29B	112.8(12)
F24B-C32B-C29B	113.3(11)
F23B-C32B-C29B	112.4(10)

Table 3. Torsion angles [°] for mo_SFCA9.

Au2-C1-C2-C3	-27(10)
Au1-C1-C2-C3	171(5)
Au2-C1-C2-Au1	162(6)
C1-C2-C3-C4	-106(5)
Au1-C2-C3-C4	63.4(13)
C1-C2-C3-C9	17(6)
Au1-C2-C3-C9	-173.2(9)
C2-C3-C4-C5	-168.6(12)
C9-C3-C4-C5	66.9(16)
C3-C4-C5-C6	-5(2)
C4-C5-C6-C7	-35(2)
C5-C6-C7-C8	1(2)
C6-C7-C8-C9	31(3)
C7-C8-C9-C3	9(2)
C4-C3-C9-C8	-69.0(17)
C2-C3-C9-C8	163.4(14)
C15-C10-C11-C12	1.6(17)
P1-C10-C11-C12	179.7(10)
C10-C11-C12-C13	-2(2)
C11-C12-C13-C14	2(2)
C12-C13-C14-C15	-0.7(19)

C13-C14-C15-C10	0.1(17)
C13-C14-C15-C16	176.6(11)
C11-C10-C15-C14	-0.5(15)
P1-C10-C15-C14	-178.5(8)
C11-C10-C15-C16	-176.6(11)
P1-C10-C15-C16	5.5(15)
C14-C15-C16-C17	79.2(13)
C10-C15-C16-C17	-104.7(13)
C14-C15-C16-C21	-94.5(13)
C10-C15-C16-C21	81.7(14)
C21-C16-C17-C18	-4.2(16)
C15-C16-C17-C18	-177.7(10)
C21-C16-C17-C22	168.6(10)
C15-C16-C17-C22	-4.9(16)
C16-C17-C18-C19	0.1(16)
C22-C17-C18-C19	-173.0(10)
C17-C18-C19-C20	2.1(15)
C17-C18-C19-C25	-179.8(10)
C18-C19-C20-C21	-0.3(15)
C25-C19-C20-C21	-178.3(10)
C19-C20-C21-C16	-3.7(17)
C19-C20-C21-C28	175.1(10)
C17-C16-C21-C20	5.9(16)
C15-C16-C21-C20	179.7(10)
C17-C16-C21-C28	-172.8(10)
C15-C16-C21-C28	1.0(16)
C16-C17-C22-C24	-101.1(12)
C18-C17-C22-C24	71.8(13)
C16-C17-C22-C23	136.9(11)
C18-C17-C22-C23	-50.3(13)
C20-C19-C25-C27	91.8(13)
C18-C19-C25-C27	-86.1(13)
C20-C19-C25-C26	-30.0(17)
C18-C19-C25-C26	152.1(11)
C20-C21-C28-C30	-84.9(13)
C16-C21-C28-C30	93.8(14)
C20-C21-C28-C29	37.7(15)
C16-C21-C28-C29	-143.6(11)

C44-C39-C40-C41	-0.7(16)
P2-C39-C40-C41	179.2(9)
C39-C40-C41-C42	2.2(18)
C40-C41-C42-C43	-1.6(18)
C41-C42-C43-C44	-0.3(19)
C42-C43-C44-C39	1.6(18)
C42-C43-C44-C45	-176.5(11)
C40-C39-C44-C43	-1.0(15)
P2-C39-C44-C43	179.0(8)
C40-C39-C44-C45	176.7(10)
P2-C39-C44-C45	-3.2(15)
C43-C44-C45-C46	-79.9(14)
C39-C44-C45-C46	102.4(14)
C43-C44-C45-C50	90.2(13)
C39-C44-C45-C50	-87.5(14)
C50-C45-C46-C47	6.1(17)
C44-C45-C46-C47	176.0(10)
C50-C45-C46-C51	-171.7(10)
C44-C45-C46-C51	-1.7(17)
C45-C46-C47-C48	-4.2(18)
C51-C46-C47-C48	173.7(11)
C46-C47-C48-C49	0.6(19)
C46-C47-C48-C54	179.7(11)
C47-C48-C49-C50	1.0(18)
C54-C48-C49-C50	-178.1(11)
C48-C49-C50-C45	1.0(18)
C48-C49-C50-C57	-174.7(12)
C46-C45-C50-C49	-4.6(17)
C44-C45-C50-C49	-174.9(10)
C46-C45-C50-C57	171.0(11)
C44-C45-C50-C57	0.7(16)
C45-C46-C51-C53	-138.5(12)
C47-C46-C51-C53	43.8(15)
C45-C46-C51-C52	97.9(13)
C47-C46-C51-C52	-79.9(14)
C49-C48-C54-C56	149.7(13)
C47-C48-C54-C56	-29.4(19)
C49-C48-C54-C55	-82.3(16)

C47-C48-C54-C55	98.6(16)
C49-C50-C57-C58	76.8(16)
C45-C50-C57-C58	-98.8(14)
C49-C50-C57-C59	-46.3(16)
C45-C50-C57-C59	138.1(12)
C11-C10-P1-C31	-68.9(10)
C15-C10-P1-C31	109.0(9)
C11-C10-P1-C35	50.9(10)
C15-C10-P1-C35	-131.2(9)
C11-C10-P1-Au1	173.0(8)
C15-C10-P1-Au1	-9.1(10)
C34-C31-P1-C10	-71.9(9)
C32-C31-P1-C10	170.7(8)
C33-C31-P1-C10	46.8(10)
C34-C31-P1-C35	171.4(8)
C32-C31-P1-C35	54.1(10)
C33-C31-P1-C35	-69.9(11)
C34-C31-P1-Au1	52.7(8)
C32-C31-P1-Au1	-64.6(9)
C33-C31-P1-Au1	171.4(8)
C40-C39-P2-C60	69.7(9)
C44-C39-P2-C60	-110.3(9)
C40-C39-P2-C64	-49.3(10)
C44-C39-P2-C64	130.7(9)
C40-C39-P2-Au2	-168.5(7)
C44-C39-P2-Au2	11.4(10)
C9B-B1B-C1B-C2B	151.0(10)
C25B-B1B-C1B-C2B	36.3(13)
C17B-B1B-C1B-C2B	-85.3(11)
C9B-B1B-C1B-C6B	-36.9(14)
C25B-B1B-C1B-C6B	-151.6(9)
C17B-B1B-C1B-C6B	86.8(11)
C6B-C1B-C2B-C3B	0.8(15)
B1B-C1B-C2B-C3B	173.5(10)
C1B-C2B-C3B-C4B	-1.1(18)
C1B-C2B-C3B-C7B	178.2(10)
C2B-C3B-C4B-C5B	-0.1(18)
C7B-C3B-C4B-C5B	-179.4(11)

C3B-C4B-C5B-C6B	1.6(18)
C3B-C4B-C5B-C8B	-179.2(11)
C4B-C5B-C6B-C1B	-2.0(17)
C8B-C5B-C6B-C1B	178.9(9)
C2B-C1B-C6B-C5B	0.8(15)
B1B-C1B-C6B-C5B	-171.7(10)
C4B-C3B-C7B-F3B	3.9(16)
C2B-C3B-C7B-F3B	-175.5(10)
C4B-C3B-C7B-F2B	126.7(12)
C2B-C3B-C7B-F2B	-52.7(14)
C4B-C3B-C7B-F1B	-116.5(12)
C2B-C3B-C7B-F1B	64.2(14)
C6B-C5B-C8B-F4B	-23(2)
C4B-C5B-C8B-F4B	158(2)
C6B-C5B-C8B-F6B"	177.5(19)
C4B-C5B-C8B-F6B"	-2(2)
C6B-C5B-C8B-F6B	102(3)
C4B-C5B-C8B-F6B	-77(3)
C6B-C5B-C8B-F6B'	139(2)
C4B-C5B-C8B-F6B'	-40(2)
C6B-C5B-C8B-F4B'	17(3)
C4B-C5B-C8B-F4B'	-162(2)
C6B-C5B-C8B-F5B"	-57(2)
C4B-C5B-C8B-F5B"	123.5(18)
C6B-C5B-C8B-F5B'	-104(2)
C4B-C5B-C8B-F5B'	77(2)
C6B-C5B-C8B-F5B	-141(2)
C4B-C5B-C8B-F5B	40(2)
C6B-C5B-C8B-F4B"	58(2)
C4B-C5B-C8B-F4B"	-120.9(19)
C1B-B1B-C9B-C10B	-37.6(15)
C25B-B1B-C9B-C10B	81.8(12)
C17B-B1B-C9B-C10B	-155.3(10)
C1B-B1B-C9B-C14B	152.0(10)
C25B-B1B-C9B-C14B	-88.6(11)
C17B-B1B-C9B-C14B	34.3(14)
C14B-C9B-C10B-C11B	1.1(16)
B1B-C9B-C10B-C11B	-169.9(10)

C9B-C10B-C11B-C12B	-0.5(17)
C9B-C10B-C11B-C15B	177.1(10)
C10B-C11B-C12B-C13B	-1.2(16)
C15B-C11B-C12B-C13B	-178.8(11)
C11B-C12B-C13B-C14B	2.3(17)
C11B-C12B-C13B-C16B	179.0(11)
C12B-C13B-C14B-C9B	-1.8(18)
C16B-C13B-C14B-C9B	-178.5(11)
C10B-C9B-C14B-C13B	0.0(16)
B1B-C9B-C14B-C13B	171.2(10)
C10B-C11B-C15B-F7B	-50.4(15)
C12B-C11B-C15B-F7B	127.2(11)
C10B-C11B-C15B-F8B	71.9(14)
C12B-C11B-C15B-F8B	-110.5(12)
C10B-C11B-C15B-F9B	-169.8(10)
C12B-C11B-C15B-F9B	7.9(16)
C12B-C13B-C16B-F10B	1.2(18)
C14B-C13B-C16B-F10B	178.0(11)
C12B-C13B-C16B-F12B	-118.8(12)
C14B-C13B-C16B-F12B	58.0(16)
C12B-C13B-C16B-F11B	122.8(12)
C14B-C13B-C16B-F11B	-60.4(15)
C1B-B1B-C17B-C22B	84.6(12)
C9B-B1B-C17B-C22B	-151.9(10)
C25B-B1B-C17B-C22B	-35.1(14)
C1B-B1B-C17B-C18B	-85.5(12)
C9B-B1B-C17B-C18B	38.0(14)
C25B-B1B-C17B-C18B	154.8(10)
C22B-C17B-C18B-C19B	0.2(16)
B1B-C17B-C18B-C19B	171.1(10)
C17B-C18B-C19B-C20B	-0.1(17)
C17B-C18B-C19B-C23B	-180.0(10)
C18B-C19B-C20B-C21B	-0.7(17)
C23B-C19B-C20B-C21B	179.1(11)
C19B-C20B-C21B-C22B	1.5(17)
C19B-C20B-C21B-C24B	179.9(11)
C20B-C21B-C22B-C17B	-1.5(18)
C24B-C21B-C22B-C17B	-179.9(11)

C18B-C17B-C22B-C21B	0.6(16)
B1B-C17B-C22B-C21B	-170.2(10)
C20B-C19B-C23B-F13B	-135.2(12)
C18B-C19B-C23B-F13B	44.6(17)
C20B-C19B-C23B-F14B	104.1(15)
C18B-C19B-C23B-F14B	-76.1(15)
C20B-C19B-C23B-F15B	-15.5(17)
C18B-C19B-C23B-F15B	164.3(12)
C20B-C21B-C24B-F16B	-113.2(13)
C22B-C21B-C24B-F16B	65.2(14)
C20B-C21B-C24B-F18B	127.5(12)
C22B-C21B-C24B-F18B	-54.1(15)
C20B-C21B-C24B-F17B	8.8(16)
C22B-C21B-C24B-F17B	-172.8(11)
C1B-B1B-C25B-C26B	-151.5(9)
C9B-B1B-C25B-C26B	87.1(11)
C17B-B1B-C25B-C26B	-36.1(14)
C1B-B1B-C25B-C30B	34.8(13)
C9B-B1B-C25B-C30B	-86.5(11)
C17B-B1B-C25B-C30B	150.3(10)
C30B-C25B-C26B-C27B	-0.7(15)
B1B-C25B-C26B-C27B	-174.8(10)
C25B-C26B-C27B-C28B	-0.8(17)
C25B-C26B-C27B-C31B	-178.6(10)
C26B-C27B-C28B-C29B	1.3(17)
C31B-C27B-C28B-C29B	179.2(10)
C27B-C28B-C29B-C30B	-0.3(18)
C27B-C28B-C29B-C32B	-179.2(11)
C28B-C29B-C30B-C25B	-1.4(18)
C32B-C29B-C30B-C25B	177.6(11)
C26B-C25B-C30B-C29B	1.8(16)
B1B-C25B-C30B-C29B	176.0(10)
C28B-C27B-C31B-F20'	-111.7(16)
C26B-C27B-C31B-F20'	66.2(17)
C28B-C27B-C31B-F19B	156.4(15)
C26B-C27B-C31B-F19B	-25.8(18)
C28B-C27B-C31B-F19'	127.5(15)
C26B-C27B-C31B-F19'	-54.7(16)

C28B-C27B-C31B-F21"	-51(3)
C26B-C27B-C31B-F21"	127(3)
C28B-C27B-C31B-F21B	32.7(17)
C26B-C27B-C31B-F21B	-149.4(14)
C28B-C27B-C31B-F21'	10.2(18)
C26B-C27B-C31B-F21'	-171.9(14)
C28B-C27B-C31B-F19"	72(3)
C26B-C27B-C31B-F19"	-110(3)
C28B-C27B-C31B-F20"	-170(2)
C26B-C27B-C31B-F20"	8(2)
C28B-C27B-C31B-F20B	-82.8(15)
C26B-C27B-C31B-F20B	95.0(14)
C30B-C29B-C32B-F22B	-155.3(11)
C28B-C29B-C32B-F22B	23.6(17)
C30B-C29B-C32B-F24B	-35.1(17)
C28B-C29B-C32B-F24B	143.8(12)
C30B-C29B-C32B-F23B	86.2(15)
C28B-C29B-C32B-F23B	-94.8(15)

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl]gold (17) CCDC 1572073.

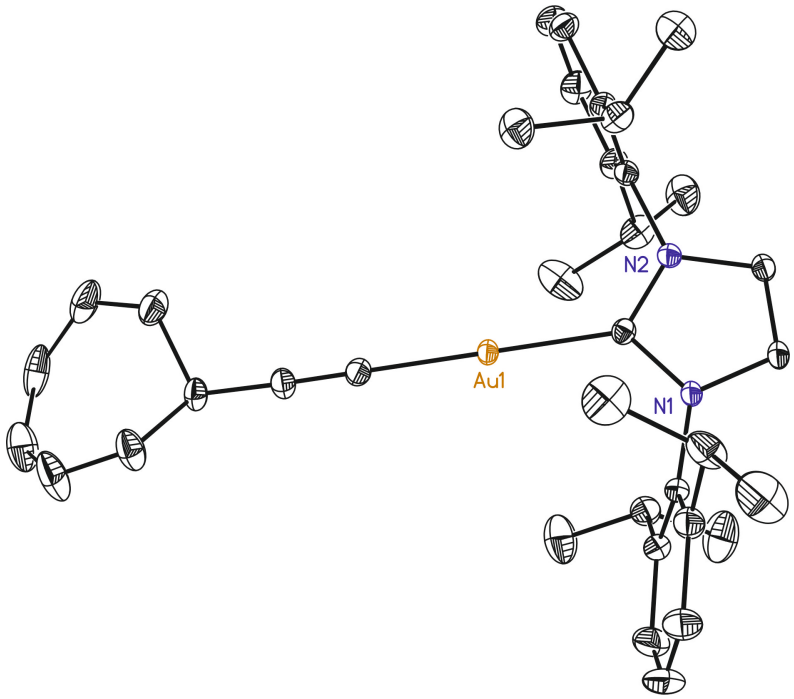


Table 1. Crystal data and structure refinement for sfc-a-5.

Identification code	sfc-a-5	
Empirical formula	C37 H45 Au Cl2 N2	
Formula weight	785.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.8291(5)Å	a= 90°.
	b = 16.8982(5)Å	b = 90°.
	c = 17.2251(6)Å	g = 90°.
Volume	3734.2(2) $Å^3$	
Z	4	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	4.108 mm^{-1}	
F(000)	1576	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	2.411 to 37.036°.	
Index ranges	-21<=h<=21,-21<=k<=28,-29<=l<=29	
Reflections collected	51198	
Independent reflections	18391[R(int) = 0.0544]	
Completeness to theta =37.036°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.494 and 0.38	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18391/ 1522/ 711	
Goodness-of-fit on F^2	0.914	
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.0818	
R indices (all data)	R1 = 0.1352, wR2 = 0.1045	
Flack parameter	x =-0.009(5)	
Largest diff. peak and hole	1.372 and -0.404 e.$Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for sfc-a-5.

Bond lengths----	
Au1-C1'	1.958(13)
Au1-C28'	1.999(6)
Au1-C28	1.999(6)

Au1-C1	2.046(12)
C1-N1	1.4200
C1-N2	1.4200
N1-C4	1.368(8)
N1-C2	1.4200
C2-C3	1.4200
C2-H2	0.9500
C3-N2	1.4200
C3-H3	0.9500
N2-C16	1.390(7)
C4-C5	1.407(9)
C4-C9	1.409(10)
C5-C6	1.418(11)
C5-C10	1.535(18)
C6-C7	1.333(15)
C6-H6	0.9500
C7-C8	1.354(15)
C7-H7	0.9500
C8-C9	1.420(11)
C8-H8	0.9500
C9-C13	1.54(2)
C10-C12	1.511(11)
C10-C11	1.511(11)
C10-H10	1.0000
C11-H11A	0.9800
C11-H11B	0.9800
C11-H11C	0.9800
C12-H12A	0.9800
C12-H12B	0.9800
C12-H12C	0.9800
C13-C15	1.42(2)
C13-C14	1.565(18)
C13-H13	1.0000
C14-H14A	0.9800
C14-H14B	0.9800
C14-H14C	0.9800
C15-H15A	0.9800
C15-H15B	0.9800

C15-H15C	0.9800
C16-C17	1.405(9)
C16-C21	1.413(9)
C17-C18	1.417(10)
C17-C22	1.470(13)
C18-C19	1.336(14)
C18-H18	0.9500
C19-C20	1.356(14)
C19-H19	0.9500
C20-C21	1.416(11)
C20-H20	0.9500
C21-C25	1.498(13)
C22-C24	1.48(3)
C22-C23	1.60(3)
C22-H22	1.0000
C23-H23A	0.9800
C23-H23B	0.9800
C23-H23C	0.9800
C24-H24A	0.9800
C24-H24B	0.9800
C24-H24C	0.9800
C25-C26	1.464(16)
C25-C27	1.468(16)
C25-H25	1.0000
C26-H26A	0.9800
C26-H26B	0.9800
C26-H26C	0.9800
C27-H27A	0.9800
C27-H27B	0.9800
C27-H27C	0.9800
C1'-N2'	1.398(6)
C1'-N1'	1.407(6)
N1'-C4'	1.376(8)
N1'-C2'	1.416(6)
C2'-C3'	1.396(6)
C2'-H2'	0.9500
C3'-N2'	1.414(6)
C3'-H3'	0.9500

N2'-C16'	1.398(7)
C4'-C5'	1.402(9)
C4'-C9'	1.414(10)
C5'-C6'	1.420(11)
C5'-C10'	1.541(18)
C6'-C7'	1.331(15)
C6'-H6'	0.9500
C7'-C8'	1.355(15)
C7'-H7'	0.9500
C8'-C9'	1.420(11)
C8'-H8'	0.9500
C9'-C13'	1.54(2)
C10'-C12'	1.516(13)
C10'-C11'	1.518(13)
C10'-H10'	1.0000
C11'-H11D	0.9800
C11'-H11E	0.9800
C11'-H11F	0.9800
C12'-H12D	0.9800
C12'-H12E	0.9800
C12'-H12F	0.9800
C13'-C15'	1.42(2)
C13'-C14'	1.562(18)
C13'-H13'	1.0000
C14'-H14D	0.9800
C14'-H14E	0.9800
C14'-H14F	0.9800
C15'-H15D	0.9800
C15'-H15E	0.9800
C15'-H15F	0.9800
C16'-C17'	1.404(9)
C16'-C21'	1.414(9)
C17'-C18'	1.420(10)
C17'-C22'	1.471(13)
C18'-C19'	1.334(14)
C18'-H18'	0.9500
C19'-C20'	1.355(14)
C19'-H19'	0.9500

C20'-C21'	1.417(11)
C20'-H20'	0.9500
C21'-C25'	1.502(13)
C22'-C24'	1.47(3)
C22'-C23'	1.60(3)
C22'-H22'	1.0000
C23'-H23D	0.9800
C23'-H23E	0.9800
C23'-H23F	0.9800
C24'-H24D	0.9800
C24'-H24E	0.9800
C24'-H24F	0.9800
C25'-C26'	1.470(16)
C25'-C27'	1.474(16)
C25'-H25'	1.0000
C26'-H26D	0.9800
C26'-H26E	0.9800
C26'-H26F	0.9800
C27'-H27D	0.9800
C27'-H27E	0.9800
C27'-H27F	0.9800
C28-C29	1.180(9)
C29-C30	1.469(10)
C30-C31	1.505(11)
C30-C36	1.515(12)
C30-H30	1.0000
C31-C32	1.348(10)
C31-H31	0.9500
C32-C33	1.441(11)
C32-H32	0.9500
C33-C34	1.319(10)
C33-H33	0.9500
C34-C35	1.427(10)
C34-H34	0.9500
C35-C36	1.343(10)
C35-H35	0.9500
C36-H36	0.9500
C28'-C29'	1.180(9)

C29'-C30'	1.465(10)
C30'-C36'	1.39(3)
C30'-C31'	1.505(12)
C30'-H30'	1.0000
C31'-C32'	1.352(11)
C31'-H31'	0.9500
C32'-C33'	1.442(12)
C32'-H32'	0.9500
C33'-C34'	1.315(11)
C33'-H33'	0.9500
C34'-C35'	1.423(12)
C34'-H34'	0.9500
C35'-C36'	1.39(2)
C35'-H35'	0.9500
C36'-H36'	0.9500
C1S-Cl1S	1.725(14)
C1S-Cl2S	1.732(14)
C1S-H1SA	0.9900
C1S-H1SB	0.9900

Angles----------

C1'-Au1-C28'	175.0(6)
C28-Au1-C1	177.1(5)
N1-C1-N2	108.0
N1-C1-Au1	124.7(7)
N2-C1-Au1	126.3(7)
C4-N1-C2	125.9(6)
C4-N1-C1	126.1(6)
C2-N1-C1	108.0
N1-C2-C3	108.0
N1-C2-H2	126.0
C3-C2-H2	126.0
N2-C3-C2	108.0
N2-C3-H3	126.0
C2-C3-H3	126.0
C16-N2-C3	124.9(6)
C16-N2-C1	124.7(6)
C3-N2-C1	108.0

N1-C4-C5	117.6(8)
N1-C4-C9	117.2(8)
C5-C4-C9	125.3(7)
C4-C5-C6	113.9(8)
C4-C5-C10	120.6(9)
C6-C5-C10	125.3(10)
C7-C6-C5	122.9(10)
C7-C6-H6	118.6
C5-C6-H6	118.6
C6-C7-C8	121.7(10)
C6-C7-H7	119.2
C8-C7-H7	119.2
C7-C8-C9	121.6(10)
C7-C8-H8	119.2
C9-C8-H8	119.2
C4-C9-C8	114.5(9)
C4-C9-C13	123.4(9)
C8-C9-C13	122.1(10)
C12-C10-C11	110.6(10)
C12-C10-C5	112.1(12)
C11-C10-C5	110.8(12)
C12-C10-H10	107.7
C11-C10-H10	107.7
C5-C10-H10	107.7
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5
C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C15-C13-C9	111.8(13)
C15-C13-C14	112.1(16)

C9-C13-C14	108.1(16)
C15-C13-H13	108.2
C9-C13-H13	108.2
C14-C13-H13	108.2
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
N2-C16-C17	117.4(7)
N2-C16-C21	118.1(7)
C17-C16-C21	124.6(7)
C16-C17-C18	114.8(8)
C16-C17-C22	121.8(8)
C18-C17-C22	123.4(9)
C19-C18-C17	122.6(9)
C19-C18-H18	118.7
C17-C18-H18	118.7
C18-C19-C20	121.1(9)
C18-C19-H19	119.5
C20-C19-H19	119.5
C19-C20-C21	122.4(10)
C19-C20-H20	118.8
C21-C20-H20	118.8
C16-C21-C20	114.4(8)
C16-C21-C25	124.4(8)
C20-C21-C25	121.2(9)
C17-C22-C24	114.2(16)
C17-C22-C23	110.4(16)
C24-C22-C23	109.3(10)
C17-C22-H22	107.6

C24-C22-H22	107.6
C23-C22-H22	107.6
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C26-C25-C27	111.6(12)
C26-C25-C21	116.1(11)
C27-C25-C21	113.1(12)
C26-C25-H25	104.9
C27-C25-H25	104.9
C21-C25-H25	104.9
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5
C25-C27-H27C	109.5
H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
N2'-C1'-N1'	105.1(5)
N2'-C1'-Au1	126.6(8)
N1'-C1'-Au1	128.2(8)
C4'-N1'-C1'	125.7(7)
C4'-N1'-C2'	123.4(7)
C1'-N1'-C2'	110.8(5)

C3'-C2'-N1'	106.1(5)
C3'-C2'-H2'	127.0
N1'-C2'-H2'	127.0
C2'-C3'-N2'	108.1(5)
C2'-C3'-H3'	126.0
N2'-C3'-H3'	126.0
C16'-N2'-C1'	125.2(7)
C16'-N2'-C3'	123.4(7)
C1'-N2'-C3'	109.9(5)
N1'-C4'-C5'	119.2(9)
N1'-C4'-C9'	115.4(8)
C5'-C4'-C9'	125.0(7)
C4'-C5'-C6'	114.3(9)
C4'-C5'-C10'	122.1(9)
C6'-C5'-C10'	123.5(10)
C7'-C6'-C5'	122.8(10)
C7'-C6'-H6'	118.6
C5'-C6'-H6'	118.6
C6'-C7'-C8'	121.6(10)
C6'-C7'-H7'	119.2
C8'-C7'-H7'	119.2
C7'-C8'-C9'	121.7(10)
C7'-C8'-H8'	119.1
C9'-C8'-H8'	119.1
C4'-C9'-C8'	114.5(9)
C4'-C9'-C13'	122.0(9)
C8'-C9'-C13'	123.0(11)
C12'-C10'-C11'	108.7(11)
C12'-C10'-C5'	111.6(13)
C11'-C10'-C5'	109.2(13)
C12'-C10'-H10'	109.1
C11'-C10'-H10'	109.1
C5'-C10'-H10'	109.1
C10'-C11'-H11D	109.5
C10'-C11'-H11E	109.5
H11D-C11'-H11E	109.5
C10'-C11'-H11F	109.5
H11D-C11'-H11F	109.5

H11E-C11'-H11F	109.5
C10'-C12'-H12D	109.5
C10'-C12'-H12E	109.5
H12D-C12'-H12E	109.5
C10'-C12'-H12F	109.5
H12D-C12'-H12F	109.5
H12E-C12'-H12F	109.5
C15'-C13'-C9'	112.5(13)
C15'-C13'-C14'	113.2(16)
C9'-C13'-C14'	108.7(16)
C15'-C13'-H13'	107.3
C9'-C13'-H13'	107.3
C14'-C13'-H13'	107.3
C13'-C14'-H14D	109.5
C13'-C14'-H14E	109.5
H14D-C14'-H14E	109.5
C13'-C14'-H14F	109.5
H14D-C14'-H14F	109.5
H14E-C14'-H14F	109.5
C13'-C15'-H15D	109.5
C13'-C15'-H15E	109.5
H15D-C15'-H15E	109.5
C13'-C15'-H15F	109.5
H15D-C15'-H15F	109.5
H15E-C15'-H15F	109.5
N2'-C16'-C17'	118.8(7)
N2'-C16'-C21'	117.0(7)
C17'-C16'-C21'	123.7(7)
C16'-C17'-C18'	115.1(8)
C16'-C17'-C22'	122.9(8)
C18'-C17'-C22'	121.7(9)
C19'-C18'-C17'	123.0(9)
C19'-C18'-H18'	118.5
C17'-C18'-H18'	118.5
C18'-C19'-C20'	120.6(9)
C18'-C19'-H19'	119.7
C20'-C19'-H19'	119.7
C19'-C20'-C21'	122.4(10)

C19'-C20'-H20'	118.8
C21'-C20'-H20'	118.8
C16'-C21'-C20'	115.0(8)
C16'-C21'-C25'	124.3(8)
C20'-C21'-C25'	120.6(9)
C17'-C22'-C24'	113.0(17)
C17'-C22'-C23'	111.4(16)
C24'-C22'-C23'	109.5(10)
C17'-C22'-H22'	107.6
C24'-C22'-H22'	107.6
C23'-C22'-H22'	107.6
C22'-C23'-H23D	109.5
C22'-C23'-H23E	109.5
H23D-C23'-H23E	109.5
C22'-C23'-H23F	109.5
H23D-C23'-H23F	109.5
H23E-C23'-H23F	109.5
C22'-C24'-H24D	109.5
C22'-C24'-H24E	109.5
H24D-C24'-H24E	109.5
C22'-C24'-H24F	109.5
H24D-C24'-H24F	109.5
H24E-C24'-H24F	109.5
C26'-C25'-C27'	110.1(12)
C26'-C25'-C21'	114.4(11)
C27'-C25'-C21'	111.9(12)
C26'-C25'-H25'	106.6
C27'-C25'-H25'	106.6
C21'-C25'-H25'	106.6
C25'-C26'-H26D	109.5
C25'-C26'-H26E	109.5
H26D-C26'-H26E	109.5
C25'-C26'-H26F	109.5
H26D-C26'-H26F	109.5
H26E-C26'-H26F	109.5
C25'-C27'-H27D	109.5
C25'-C27'-H27E	109.5
H27D-C27'-H27E	109.5

C25'-C27'-H27F	109.5
H27D-C27'-H27F	109.5
H27E-C27'-H27F	109.5
C29-C28-Au1	172.1(7)
C28-C29-C30	174.3(10)
C29-C30-C31	112.6(11)
C29-C30-C36	112.7(13)
C31-C30-C36	111.5(10)
C29-C30-H30	106.5
C31-C30-H30	106.5
C36-C30-H30	106.5
C32-C31-C30	122.2(10)
C32-C31-H31	118.9
C30-C31-H31	118.9
C31-C32-C33	125.6(9)
C31-C32-H32	117.2
C33-C32-H32	117.2
C34-C33-C32	128.4(11)
C34-C33-H33	115.8
C32-C33-H33	115.8
C33-C34-C35	129.4(11)
C33-C34-H34	115.3
C35-C34-H34	115.3
C36-C35-C34	127.4(10)
C36-C35-H35	116.3
C34-C35-H35	116.3
C35-C36-C30	121.8(11)
C35-C36-H36	119.1
C30-C36-H36	119.1
C29'-C28'-Au1	172.1(7)
C28'-C29'-C30'	179.5(12)
C36'-C30'-C29'	118.2(16)
C36'-C30'-C31'	119.6(16)
C29'-C30'-C31'	112.1(11)
C36'-C30'-H30'	100.6
C29'-C30'-H30'	100.6
C31'-C30'-H30'	100.6
C32'-C31'-C30'	121.6(12)

C32'-C31'-H31'	119.2
C30'-C31'-H31'	119.2
C31'-C32'-C33'	123.3(12)
C31'-C32'-H32'	118.3
C33'-C32'-H32'	118.3
C34'-C33'-C32'	128.4(15)
C34'-C33'-H33'	115.8
C32'-C33'-H33'	115.8
C33'-C34'-C35'	130.8(15)
C33'-C34'-H34'	114.6
C35'-C34'-H34'	114.6
C36'-C35'-C34'	121.8(16)
C36'-C35'-H35'	119.1
C34'-C35'-H35'	119.1
C35'-C36'-C30'	126(2)
C35'-C36'-H36'	117.2
C30'-C36'-H36'	117.2
Cl1S-C1S-Cl2S	111.8(7)
Cl1S-C1S-H1SA	109.3
Cl2S-C1S-H1SA	109.3
Cl1S-C1S-H1SB	109.3
Cl2S-C1S-H1SB	109.3
H1SA-C1S-H1SB	107.9

Table 3. Torsion angles [°] for sfc-a-5.

N2-C1-N1-C4	-178.5(12)
Au1-C1-N1-C4	-9.3(13)
N2-C1-N1-C2	0.0
Au1-C1-N1-C2	169.2(13)
C4-N1-C2-C3	178.5(12)
C1-N1-C2-C3	0.0
N1-C2-C3-N2	0.0
C2-C3-N2-C16	-162.7(11)
C2-C3-N2-C1	0.0
N1-C1-N2-C16	162.8(11)
Au1-C1-N2-C16	-6.2(15)
N1-C1-N2-C3	0.0

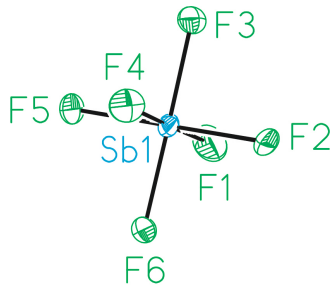
Au1-C1-N2-C3	-169.0(13)
C2-N1-C4-C5	-89.8(17)
C1-N1-C4-C5	88.4(16)
C2-N1-C4-C9	90.3(17)
C1-N1-C4-C9	-91.4(15)
N1-C4-C5-C6	-177.9(14)
C9-C4-C5-C6	2(3)
N1-C4-C5-C10	-3(2)
C9-C4-C5-C10	177.0(15)
C4-C5-C6-C7	-4(3)
C10-C5-C6-C7	-179.1(18)
C5-C6-C7-C8	3(3)
C6-C7-C8-C9	2(4)
N1-C4-C9-C8	-178.1(16)
C5-C4-C9-C8	2(3)
N1-C4-C9-C13	0(2)
C5-C4-C9-C13	-179.3(17)
C7-C8-C9-C4	-4(3)
C7-C8-C9-C13	177(2)
C4-C5-C10-C12	120.0(18)
C6-C5-C10-C12	-66(2)
C4-C5-C10-C11	-116.0(18)
C6-C5-C10-C11	58(2)
C4-C9-C13-C15	101(2)
C8-C9-C13-C15	-81(2)
C4-C9-C13-C14	-135.4(18)
C8-C9-C13-C14	43(2)
C3-N2-C16-C17	-99(2)
C1-N2-C16-C17	101(2)
C3-N2-C16-C21	81(2)
C1-N2-C16-C21	-79(2)
N2-C16-C17-C18	177.3(18)
C21-C16-C17-C18	-2(4)
N2-C16-C17-C22	-4(3)
C21-C16-C17-C22	177(2)
C16-C17-C18-C19	-1(4)
C22-C17-C18-C19	-180(2)
C17-C18-C19-C20	2(4)

C18-C19-C20-C21	-1(3)
N2-C16-C21-C20	-175.9(16)
C17-C16-C21-C20	4(4)
N2-C16-C21-C25	4(3)
C17-C16-C21-C25	-176(2)
C19-C20-C21-C16	-2(3)
C19-C20-C21-C25	177.6(18)
C16-C17-C22-C24	129(3)
C18-C17-C22-C24	-52(3)
C16-C17-C22-C23	-107(3)
C18-C17-C22-C23	72(3)
C16-C21-C25-C26	117(3)
C20-C21-C25-C26	-63(2)
C16-C21-C25-C27	-112(3)
C20-C21-C25-C27	68(2)
N2'-C1'-N1'-C4'	-176.7(12)
Au1-C1'-N1'-C4'	7(2)
N2'-C1'-N1'-C2'	-0.5(15)
Au1-C1'-N1'-C2'	-177.2(14)
C4'-N1'-C2'-C3'	175.3(13)
C1'-N1'-C2'-C3'	-1.1(17)
N1'-C2'-C3'-N2'	2.2(16)
N1'-C1'-N2'-C16'	-164.6(11)
Au1-C1'-N2'-C16'	12(2)
N1'-C1'-N2'-C3'	1.8(14)
Au1-C1'-N2'-C3'	178.6(15)
C2'-C3'-N2'-C16'	164.1(12)
C2'-C3'-N2'-C1'	-2.6(15)
C1'-N1'-C4'-C5'	82(2)
C2'-N1'-C4'-C5'	-93.9(18)
C1'-N1'-C4'-C9'	-105.2(17)
C2'-N1'-C4'-C9'	79.0(18)
N1'-C4'-C5'-C6'	173.6(15)
C9'-C4'-C5'-C6'	1(3)
N1'-C4'-C5'-C10'	-8(2)
C9'-C4'-C5'-C10'	179.7(16)
C4'-C5'-C6'-C7'	1(3)
C10'-C5'-C6'-C7'	-177(2)

C5'-C6'-C7'-C8'	-2(4)
C6'-C7'-C8'-C9'	-1(4)
N1'-C4'-C9'-C8'	-175.8(15)
C5'-C4'-C9'-C8'	-3(3)
N1'-C4'-C9'-C13'	12(2)
C5'-C4'-C9'-C13'	-175.9(16)
C7'-C8'-C9'-C4'	3(3)
C7'-C8'-C9'-C13'	175(2)
C4'-C5'-C10'-C12'	-114.9(19)
C6'-C5'-C10'-C12'	63(2)
C4'-C5'-C10'-C11'	124.9(19)
C6'-C5'-C10'-C11'	-57(2)
C4'-C9'-C13'-C15'	87(2)
C8'-C9'-C13'-C15'	-85(2)
C4'-C9'-C13'-C14'	-146.5(18)
C8'-C9'-C13'-C14'	42(2)
C1'-N2'-C16'-C17'	88(2)
C3'-N2'-C16'-C17'	-76(2)
C1'-N2'-C16'-C21'	-100(2)
C3'-N2'-C16'-C21'	96(2)
N2'-C16'-C17'-C18'	175.9(18)
C21'-C16'-C17'-C18'	4(4)
N2'-C16'-C17'-C22'	-10(4)
C21'-C16'-C17'-C22'	178(3)
C16'-C17'-C18'-C19'	-2(4)
C22'-C17'-C18'-C19'	-176(2)
C17'-C18'-C19'-C20'	1(3)
C18'-C19'-C20'-C21'	-2(3)
N2'-C16'-C21'-C20'	-176.8(17)
C17'-C16'-C21'-C20'	-5(4)
N2'-C16'-C21'-C25'	7(3)
C17'-C16'-C21'-C25'	179(2)
C19'-C20'-C21'-C16'	4(3)
C19'-C20'-C21'-C25'	-180.0(19)
C16'-C17'-C22'-C24'	-97(3)
C18'-C17'-C22'-C24'	76(3)
C16'-C17'-C22'-C23'	139(3)
C18'-C17'-C22'-C23'	-48(3)

C16'-C21'-C25'-C26'	113(3)
C20'-C21'-C25'-C26'	-63(2)
C16'-C21'-C25'-C27'	-121(2)
C20'-C21'-C25'-C27'	63(2)
C29-C30-C31-C32	-165.8(19)
C36-C30-C31-C32	66(2)
C30-C31-C32-C33	-22(3)
C31-C32-C33-C34	-17(4)
C32-C33-C34-C35	6(5)
C33-C34-C35-C36	12(5)
C34-C35-C36-C30	18(3)
C29-C30-C36-C35	169.9(18)
C31-C30-C36-C35	-62(2)
C36'-C30'-C31'-C32'	-53(3)
C29'-C30'-C31'-C32'	161.9(19)
C30'-C31'-C32'-C33'	1(4)
C31'-C32'-C33'-C34'	37(4)
C32'-C33'-C34'-C35'	-17(5)
C33'-C34'-C35'-C36'	-12(4)
C34'-C35'-C36'-C30'	-11(4)
C29'-C30'-C36'-C35'	-160.8(19)
C31'-C30'-C36'-C35'	56(3)

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (18a) CCDC 1572065.



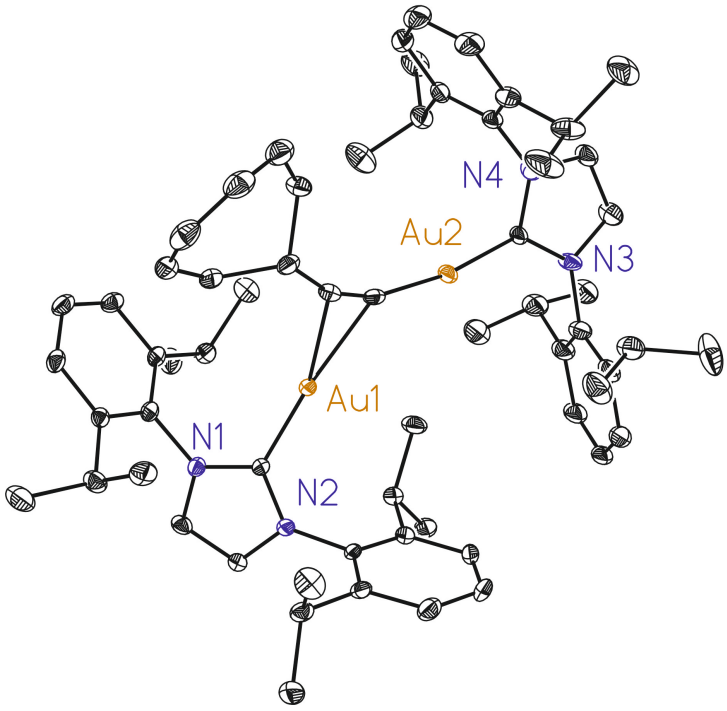


Table 1. Crystal data and structure refinement for SFC-A-10.

Identification code	SFC-A-10	
Empirical formula	C66.50 H86 Au2 Cl3 F6 N4 Sb	
Formula weight	1677.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.4152(4)Å	a= 85.700(2)°.
	b = 16.6081(4)Å	b = 74.570(2)°.
	c = 17.4949(4)Å	g = 89.181(2)°.
Volume	3467.45(16) $Å^3$	
Z	2	
Density (calculated)	1.607 Mg/m^3	
Absorption coefficient	4.779 mm^{-1}	

F(000)	1654
Crystal size	0.2 x 0.2 x 0.1 mm^3
Theta range for data collection	2.336 to 40.073°.
Index ranges	-22<=h<=22,-29<=k<=29,-31<=l<=18
Reflections collected	82972
Independent reflections	38756[R(int) = 0.0893]
Completeness to theta =40.073°	89.700005%
Absorption correction	Multi-scan
Max. and min. transmission	0.646 and 0.497
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	38756/ 278/ 892
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0795, wR2 = 0.2101
R indices (all data)	R1 = 0.1835, wR2 = 0.2470
Largest diff. peak and hole	4.500 and -3.369 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for SFC-A-10.

Bond lengths----	
C1-N1	1.359(9)
C1-N2	1.360(8)
C1-Au1	1.987(7)
N1-C2	1.375(9)
N1-C4	1.455(9)
Au1-C29	2.204(7)
Au1-C28	2.204(7)
C2-C3	1.353(11)
C2-H2	0.9300
N2-C3	1.389(9)
N2-C16	1.443(9)
Au2-C37	1.989(7)
Au2-C28	1.996(8)
C3-H3	0.9300
N3-C37	1.371(9)
N3-C38	1.387(10)
N3-C40	1.450(9)
N4-C37	1.349(9)
N4-C39	1.392(10)
N4-C52	1.441(9)

C4-C5	1.382(10)
C4-C9	1.411(10)
C5-C6	1.412(10)
C5-C10	1.511(11)
C6-C7	1.388(13)
C6-H6	0.9300
C7-C8	1.377(12)
C7-H7	0.9300
C8-C9	1.403(10)
C8-H8	0.9300
C9-C13	1.524(11)
C10-C12	1.529(13)
C10-C11	1.540(12)
C10-H10	0.9800
C11-H11A	0.9600
C11-H11B	0.9600
C11-H11C	0.9600
C12-H12A	0.9600
C12-H12B	0.9600
C12-H12C	0.9600
C13-C15	1.515(13)
C13-C14	1.519(13)
C13-H13	0.9800
C14-H14A	0.9600
C14-H14B	0.9600
C14-H14C	0.9600
C15-H15A	0.9600
C15-H15B	0.9600
C15-H15C	0.9600
C16-C21	1.376(11)
C16-C17	1.414(12)
C17-C18	1.397(11)
C17-C22	1.488(12)
C18-C19	1.414(14)
C18-H18	0.9300
C19-C20	1.341(14)
C19-H19	0.9300
C20-C21	1.394(11)

C20-H20	0.9300
C21-C25	1.539(14)
C22-C24	1.531(12)
C22-C23	1.542(13)
C22-H22	0.9800
C23-H23A	0.9600
C23-H23B	0.9600
C23-H23C	0.9600
C24-H24A	0.9600
C24-H24B	0.9600
C24-H24C	0.9600
C25-C26	1.523(10)
C25-C27	1.525(12)
C25-H25	0.9800
C26-H26A	0.9600
C26-H26B	0.9600
C26-H26C	0.9600
C27-H27A	0.9600
C27-H27B	0.9600
C27-H27C	0.9600
C28-C29	1.235(11)
C29-C30	1.455(11)
C30-C36	1.485(12)
C30-C31	1.497(10)
C30-H30	0.9800
C31-C32	1.319(14)
C31-H31	0.9300
C32-C33	1.440(16)
C32-H32	0.9300
C33-C34	1.345(16)
C33-H33	0.9300
C34-C35	1.433(16)
C34-H34	0.9300
C35-C36	1.326(13)
C35-H35	0.9300
C36-H36	0.9300
C38-C39	1.360(12)
C38-H38	0.9300

C39-H39	0.9300
C40-C45	1.409(15)
C40-C41	1.415(15)
C41-C42	1.409(12)
C41-C46	1.442(17)
C42-C43	1.437(16)
C42-H42	0.9300
C43-C44	1.360(16)
C43-H43	0.9300
C44-C45	1.381(12)
C44-H44	0.9300
C45-C49	1.543(16)
C46-C48	1.508(15)
C46-C47	1.590(17)
C46-H46	0.9800
C47-H47A	0.9600
C47-H47B	0.9600
C47-H47C	0.9600
C48-H48A	0.9600
C48-H48B	0.9600
C48-H48C	0.9600
C49-C51	1.526(14)
C49-C50	1.527(16)
C49-H49	0.9800
C50-H50A	0.9600
C50-H50B	0.9600
C50-H50C	0.9600
C51-H51A	0.9600
C51-H51B	0.9600
C51-H51C	0.9600
C52-C57	1.382(12)
C52-C53	1.418(12)
C53-C54	1.414(12)
C53-C58	1.524(13)
C54-C55	1.383(15)
C54-H54	0.9300
C55-C56	1.332(15)
C55-H55	0.9300

C56-C57	1.384(12)
C56-H56	0.9300
C57-C61	1.532(15)
C58-C60	1.517(14)
C58-C59	1.547(15)
C58-H58	0.9800
C59-H59A	0.9600
C59-H59B	0.9600
C59-H59C	0.9600
C60-H60A	0.9600
C60-H60B	0.9600
C60-H60C	0.9600
C61-C63	1.477(18)
C61-C62	1.589(14)
C61-H61	0.9800
C62-H62A	0.9600
C62-H62B	0.9600
C62-H62C	0.9600
C63-H63A	0.9600
C63-H63B	0.9600
C63-H63C	0.9600
C1S-Cl2S	1.718(9)
C1S-Cl3S	1.744(10)
C1S-Cl1S	1.794(9)
C1S-H1S	0.9800
Sb1-F1	1.831(9)
Sb1-F6	1.850(6)
Sb1-F3	1.852(5)
Sb1-F5	1.864(6)
Sb1-F4	1.882(8)
Sb1-F2	1.895(7)
Sb1'-F1'	1.834(10)
Sb1'-F6'	1.850(7)
Sb1'-F3'	1.853(6)
Sb1'-F5'	1.864(7)
Sb1'-F4'	1.880(9)
Sb1'-F2'	1.894(8)
C1H-C2H	1.539(5)

C1H-H1H1	0.9600
C1H-H1H2	0.9600
C1H-H1H3	0.9600
C2H-C3H	1.538(5)
C2H-H2H1	0.9700
C2H-H2H2	0.9700
C3H-C4H	1.539(5)
C3H-H3H1	0.9700
C3H-H3H2	0.9700
C4H-C5H	1.539(5)
C4H-H4H1	0.9700
C4H-H4H2	0.9700
C5H-H5H1	0.9600
C5H-H5H2	0.9600
C5H-H5H3	0.9600
C1H'-C2H'	1.539(7)
C1H'-H1'1	0.9600
C1H'-H1'2	0.9600
C1H'-H1'3	0.9600
C2H'-C3H'	1.536(7)
C2H'-H2'1	0.9700
C2H'-H2'2	0.9700
C3H'-C4H'	1.538(7)
C3H'-H3'1	0.9700
C3H'-H3'2	0.9700
C4H'-C5H'	1.539(7)
C4H'-H4'1	0.9700
C4H'-H4'2	0.9700
C5H'-H5'1	0.9600
C5H'-H5'2	0.9600
C5H'-H5'3	0.9600

Angles----------

N1-C1-N2	104.1(6)
N1-C1-Au1	124.8(5)
N2-C1-Au1	130.7(5)
C1-N1-C2	111.8(6)
C1-N1-C4	123.1(6)

C2-N1-C4	125.1(6)
C1-Au1-C29	162.5(3)
C1-Au1-C28	163.1(3)
C29-Au1-C28	32.5(3)
C3-C2-N1	106.5(7)
C3-C2-H2	126.8
N1-C2-H2	126.8
C1-N2-C3	110.9(6)
C1-N2-C16	123.1(6)
C3-N2-C16	126.0(6)
C37-Au2-C28	169.0(3)
C2-C3-N2	106.8(6)
C2-C3-H3	126.6
N2-C3-H3	126.6
C37-N3-C38	111.9(6)
C37-N3-C40	126.6(6)
C38-N3-C40	121.4(6)
C37-N4-C39	113.1(6)
C37-N4-C52	124.3(6)
C39-N4-C52	122.5(6)
C5-C4-C9	124.8(7)
C5-C4-N1	117.3(6)
C9-C4-N1	117.9(6)
C4-C5-C6	116.4(7)
C4-C5-C10	123.8(7)
C6-C5-C10	119.8(7)
C7-C6-C5	120.2(8)
C7-C6-H6	119.9
C5-C6-H6	119.9
C8-C7-C6	122.0(7)
C8-C7-H7	119.0
C6-C7-H7	119.0
C7-C8-C9	120.1(7)
C7-C8-H8	120.0
C9-C8-H8	120.0
C8-C9-C4	116.5(7)
C8-C9-C13	121.3(7)
C4-C9-C13	122.1(6)

C5-C10-C12	110.0(7)
C5-C10-C11	113.3(7)
C12-C10-C11	109.7(8)
C5-C10-H10	107.9
C12-C10-H10	107.9
C11-C10-H10	107.9
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5
C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C15-C13-C14	109.4(8)
C15-C13-C9	113.6(8)
C14-C13-C9	109.8(6)
C15-C13-H13	108.0
C14-C13-H13	108.0
C9-C13-H13	108.0
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C21-C16-C17	123.4(7)
C21-C16-N2	119.7(7)

C17-C16-N2	116.8(7)
C18-C17-C16	115.7(8)
C18-C17-C22	120.6(8)
C16-C17-C22	123.7(7)
C17-C18-C19	120.8(9)
C17-C18-H18	119.6
C19-C18-H18	119.6
C20-C19-C18	121.0(8)
C20-C19-H19	119.5
C18-C19-H19	119.5
C19-C20-C21	120.6(9)
C19-C20-H20	119.7
C21-C20-H20	119.7
C16-C21-C20	118.4(9)
C16-C21-C25	121.8(7)
C20-C21-C25	119.7(8)
C17-C22-C24	113.0(7)
C17-C22-C23	111.3(7)
C24-C22-C23	109.6(8)
C17-C22-H22	107.6
C24-C22-H22	107.6
C23-C22-H22	107.6
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C26-C25-C27	111.0(7)
C26-C25-C21	111.7(8)
C27-C25-C21	112.8(7)
C26-C25-H25	107.0

C27-C25-H25	107.0
C21-C25-H25	107.0
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5
C25-C27-H27C	109.5
H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
C29-C28-Au2	162.4(6)
C29-C28-Au1	73.7(4)
Au2-C28-Au1	123.2(4)
C28-C29-C30	160.3(7)
C28-C29-Au1	73.7(5)
C30-C29-Au1	126.0(5)
C29-C30-C36	115.2(7)
C29-C30-C31	112.2(7)
C36-C30-C31	108.3(6)
C29-C30-H30	106.9
C36-C30-H30	106.9
C31-C30-H30	106.9
C32-C31-C30	120.7(9)
C32-C31-H31	119.6
C30-C31-H31	119.6
C31-C32-C33	124.8(9)
C31-C32-H32	117.6
C33-C32-H32	117.6
C34-C33-C32	124.8(10)
C34-C33-H33	117.6
C32-C33-H33	117.6
C33-C34-C35	125.8(10)
C33-C34-H34	117.1
C35-C34-H34	117.1

C36-C35-C34	125.9(9)
C36-C35-H35	117.0
C34-C35-H35	117.0
C35-C36-C30	120.7(9)
C35-C36-H36	119.6
C30-C36-H36	119.6
N4-C37-N3	102.9(6)
N4-C37-Au2	122.3(5)
N3-C37-Au2	133.7(5)
C39-C38-N3	106.6(7)
C39-C38-H38	126.7
N3-C38-H38	126.7
C38-C39-N4	105.4(7)
C38-C39-H39	127.3
N4-C39-H39	127.3
C45-C40-C41	125.4(8)
C45-C40-N3	117.5(9)
C41-C40-N3	117.0(9)
C42-C41-C40	115.9(10)
C42-C41-C46	119.7(11)
C40-C41-C46	124.4(8)
C41-C42-C43	118.9(11)
C41-C42-H42	120.5
C43-C42-H42	120.5
C44-C43-C42	121.8(8)
C44-C43-H43	119.1
C42-C43-H43	119.1
C43-C44-C45	122.0(10)
C43-C44-H44	119.0
C45-C44-H44	119.0
C44-C45-C40	116.0(11)
C44-C45-C49	120.2(10)
C40-C45-C49	123.8(8)
C41-C46-C48	112.7(9)
C41-C46-C47	112.6(9)
C48-C46-C47	107.0(12)
C41-C46-H46	108.1
C48-C46-H46	108.1

C47-C46-H46	108.1
C46-C47-H47A	109.5
C46-C47-H47B	109.5
H47A-C47-H47B	109.5
C46-C47-H47C	109.5
H47A-C47-H47C	109.5
H47B-C47-H47C	109.5
C46-C48-H48A	109.5
C46-C48-H48B	109.5
H48A-C48-H48B	109.5
C46-C48-H48C	109.5
H48A-C48-H48C	109.5
H48B-C48-H48C	109.5
C51-C49-C50	110.6(10)
C51-C49-C45	109.3(9)
C50-C49-C45	112.4(9)
C51-C49-H49	108.1
C50-C49-H49	108.1
C45-C49-H49	108.1
C49-C50-H50A	109.5
C49-C50-H50B	109.5
H50A-C50-H50B	109.5
C49-C50-H50C	109.5
H50A-C50-H50C	109.5
H50B-C50-H50C	109.5
C49-C51-H51A	109.5
C49-C51-H51B	109.5
H51A-C51-H51B	109.5
C49-C51-H51C	109.5
H51A-C51-H51C	109.5
H51B-C51-H51C	109.5
C57-C52-C53	122.6(7)
C57-C52-N4	121.5(8)
C53-C52-N4	115.9(7)
C54-C53-C52	116.2(8)
C54-C53-C58	119.8(8)
C52-C53-C58	123.9(7)
C55-C54-C53	120.2(9)

C55-C54-H54	119.9
C53-C54-H54	119.9
C56-C55-C54	121.1(9)
C56-C55-H55	119.4
C54-C55-H55	119.4
C55-C56-C57	122.5(9)
C55-C56-H56	118.8
C57-C56-H56	118.8
C52-C57-C56	117.4(9)
C52-C57-C61	120.1(7)
C56-C57-C61	122.5(8)
C60-C58-C53	110.9(9)
C60-C58-C59	110.7(9)
C53-C58-C59	113.8(7)
C60-C58-H58	107.0
C53-C58-H58	107.0
C59-C58-H58	107.0
C58-C59-H59A	109.5
C58-C59-H59B	109.5
H59A-C59-H59B	109.5
C58-C59-H59C	109.5
H59A-C59-H59C	109.5
H59B-C59-H59C	109.5
C58-C60-H60A	109.5
C58-C60-H60B	109.5
H60A-C60-H60B	109.5
C58-C60-H60C	109.5
H60A-C60-H60C	109.5
H60B-C60-H60C	109.5
C63-C61-C57	110.5(11)
C63-C61-C62	109.5(9)
C57-C61-C62	108.9(8)
C63-C61-H61	109.3
C57-C61-H61	109.3
C62-C61-H61	109.3
C61-C62-H62A	109.5
C61-C62-H62B	109.5
H62A-C62-H62B	109.5

C61-C62-H62C	109.5
H62A-C62-H62C	109.5
H62B-C62-H62C	109.5
C61-C63-H63A	109.5
C61-C63-H63B	109.5
H63A-C63-H63B	109.5
C61-C63-H63C	109.5
H63A-C63-H63C	109.5
H63B-C63-H63C	109.5
Cl2S-C1S-Cl3S	113.5(5)
Cl2S-C1S-Cl1S	111.2(5)
Cl3S-C1S-Cl1S	110.8(5)
Cl2S-C1S-H1S	107.0
Cl3S-C1S-H1S	107.0
Cl1S-C1S-H1S	107.0
F1-Sb1-F6	88.8(4)
F1-Sb1-F3	90.8(4)
F6-Sb1-F3	179.1(3)
F1-Sb1-F5	92.7(4)
F6-Sb1-F5	88.9(3)
F3-Sb1-F5	90.2(3)
F1-Sb1-F4	178.1(4)
F6-Sb1-F4	91.6(4)
F3-Sb1-F4	88.7(3)
F5-Sb1-F4	89.1(3)
F1-Sb1-F2	91.7(4)
F6-Sb1-F2	90.9(3)
F3-Sb1-F2	90.0(3)
F5-Sb1-F2	175.6(4)
F4-Sb1-F2	86.5(4)
F1'-Sb1'-F6'	88.5(5)
F1'-Sb1'-F3'	90.7(5)
F6'-Sb1'-F3'	178.8(6)
F1'-Sb1'-F5'	92.4(6)
F6'-Sb1'-F5'	89.1(5)
F3'-Sb1'-F5'	90.0(4)
F1'-Sb1'-F4'	178.5(6)
F6'-Sb1'-F4'	91.7(5)

F3'-Sb1'-F4'	89.0(5)
F5'-Sb1'-F4'	89.1(5)
F1'-Sb1'-F2'	91.9(5)
F6'-Sb1'-F2'	91.1(5)
F3'-Sb1'-F2'	89.8(4)
F5'-Sb1'-F2'	175.7(6)
F4'-Sb1'-F2'	86.6(6)
C2H-C1H-H1H1	109.5
C2H-C1H-H1H2	109.5
H1H1-C1H-H1H2	109.5
C2H-C1H-H1H3	109.5
H1H1-C1H-H1H3	109.5
H1H2-C1H-H1H3	109.5
C3H-C2H-C1H	109.0(7)
C3H-C2H-H2H1	109.9
C1H-C2H-H2H1	109.9
C3H-C2H-H2H2	109.9
C1H-C2H-H2H2	109.9
H2H1-C2H-H2H2	108.3
C2H-C3H-C4H	108.9(7)
C2H-C3H-H3H1	109.9
C4H-C3H-H3H1	109.9
C2H-C3H-H3H2	109.9
C4H-C3H-H3H2	109.9
H3H1-C3H-H3H2	108.3
C3H-C4H-C5H	108.7(7)
C3H-C4H-H4H1	109.9
C5H-C4H-H4H1	109.9
C3H-C4H-H4H2	109.9
C5H-C4H-H4H2	109.9
H4H1-C4H-H4H2	108.3
C4H-C5H-H5H1	109.5
C4H-C5H-H5H2	109.5
H5H1-C5H-H5H2	109.5
C4H-C5H-H5H3	109.5
H5H1-C5H-H5H3	109.5
H5H2-C5H-H5H3	109.5
C2H'-C1H'-H1'1	109.5

C2H'-C1H'-H1'2	109.5
H1'1-C1H'-H1'2	109.5
C2H'-C1H'-H1'3	109.4
H1'1-C1H'-H1'3	109.5
H1'2-C1H'-H1'3	109.5
C3H'-C2H'-C1H'	109.0(10)
C3H'-C2H'-H2'1	109.9
C1H'-C2H'-H2'1	109.9
C3H'-C2H'-H2'2	109.9
C1H'-C2H'-H2'2	109.9
H2'1-C2H'-H2'2	108.3
C2H'-C3H'-C4H'	109.3(9)
C2H'-C3H'-H3'1	109.8
C4H'-C3H'-H3'1	109.8
C2H'-C3H'-H3'2	109.8
C4H'-C3H'-H3'2	109.8
H3'1-C3H'-H3'2	108.3
C3H'-C4H'-C5H'	108.7(10)
C3H'-C4H'-H4'1	110.0
C5H'-C4H'-H4'1	110.0
C3H'-C4H'-H4'2	110.0
C5H'-C4H'-H4'2	110.0
H4'1-C4H'-H4'2	108.3
C4H'-C5H'-H5'1	109.4
C4H'-C5H'-H5'2	109.5
H5'1-C5H'-H5'2	109.5
C4H'-C5H'-H5'3	109.5
H5'1-C5H'-H5'3	109.5
H5'2-C5H'-H5'3	109.5

Table 3. Torsion angles [°] for SFC-A-10.

N2-C1-N1-C2	0.1(8)
Au1-C1-N1-C2	173.2(6)
N2-C1-N1-C4	178.9(6)
Au1-C1-N1-C4	-8.1(10)
C1-N1-C2-C3	-1.3(9)
C4-N1-C2-C3	-180.0(7)

N1-C1-N2-C3	1.1(8)
Au1-C1-N2-C3	-171.4(6)
N1-C1-N2-C16	-175.5(7)
Au1-C1-N2-C16	12.0(11)
N1-C2-C3-N2	1.8(9)
C1-N2-C3-C2	-1.9(9)
C16-N2-C3-C2	174.6(7)
C1-N1-C4-C5	80.5(9)
C2-N1-C4-C5	-101.0(9)
C1-N1-C4-C9	-98.5(8)
C2-N1-C4-C9	80.0(9)
C9-C4-C5-C6	0.8(11)
N1-C4-C5-C6	-178.1(6)
C9-C4-C5-C10	-178.0(7)
N1-C4-C5-C10	3.0(11)
C4-C5-C6-C7	-0.7(11)
C10-C5-C6-C7	178.2(7)
C5-C6-C7-C8	0.2(12)
C6-C7-C8-C9	0.3(12)
C7-C8-C9-C4	-0.2(11)
C7-C8-C9-C13	178.3(7)
C5-C4-C9-C8	-0.3(11)
N1-C4-C9-C8	178.6(6)
C5-C4-C9-C13	-178.9(7)
N1-C4-C9-C13	0.0(10)
C4-C5-C10-C12	106.5(9)
C6-C5-C10-C12	-72.4(9)
C4-C5-C10-C11	-130.4(8)
C6-C5-C10-C11	50.8(10)
C8-C9-C13-C15	32.8(11)
C4-C9-C13-C15	-148.7(8)
C8-C9-C13-C14	-90.1(9)
C4-C9-C13-C14	88.4(9)
C1-N2-C16-C21	-90.0(9)
C3-N2-C16-C21	94.0(9)
C1-N2-C16-C17	87.5(8)
C3-N2-C16-C17	-88.6(9)
C21-C16-C17-C18	1.8(11)

N2-C16-C17-C18	-175.5(6)
C21-C16-C17-C22	-176.9(7)
N2-C16-C17-C22	5.7(10)
C16-C17-C18-C19	-0.2(11)
C22-C17-C18-C19	178.6(8)
C17-C18-C19-C20	-0.3(13)
C18-C19-C20-C21	-0.7(13)
C17-C16-C21-C20	-2.9(11)
N2-C16-C21-C20	174.4(6)
C17-C16-C21-C25	179.6(7)
N2-C16-C21-C25	-3.1(10)
C19-C20-C21-C16	2.2(11)
C19-C20-C21-C25	179.8(7)
C18-C17-C22-C24	-63.7(11)
C16-C17-C22-C24	115.0(9)
C18-C17-C22-C23	60.1(10)
C16-C17-C22-C23	-121.2(9)
C16-C21-C25-C26	102.8(8)
C20-C21-C25-C26	-74.7(9)
C16-C21-C25-C27	-131.4(8)
C20-C21-C25-C27	51.1(10)
Au2-C28-C29-C30	-12(4)
Au1-C28-C29-C30	-176(2)
Au2-C28-C29-Au1	165(2)
C28-C29-C30-C36	142(2)
Au1-C29-C30-C36	-33.1(10)
C28-C29-C30-C31	18(3)
Au1-C29-C30-C31	-157.7(6)
C29-C30-C31-C32	-163.1(9)
C36-C30-C31-C32	68.6(12)
C30-C31-C32-C33	-6.8(16)
C31-C32-C33-C34	-36.7(17)
C32-C33-C34-C35	6.5(17)
C33-C34-C35-C36	28.6(16)
C34-C35-C36-C30	7.1(14)
C29-C30-C36-C35	166.4(8)
C31-C30-C36-C35	-67.0(10)
C39-N4-C37-N3	2.2(11)

C52-N4-C37-N3	-174.5(8)
C39-N4-C37-Au2	171.8(7)
C52-N4-C37-Au2	-4.9(12)
C38-N3-C37-N4	-1.7(11)
C40-N3-C37-N4	-177.7(9)
C38-N3-C37-Au2	-169.6(8)
C40-N3-C37-Au2	14.5(15)
C37-N3-C38-C39	0.7(12)
C40-N3-C38-C39	176.9(10)
N3-C38-C39-N4	0.7(12)
C37-N4-C39-C38	-1.9(12)
C52-N4-C39-C38	174.9(9)
C37-N3-C40-C45	101.2(11)
C38-N3-C40-C45	-74.4(12)
C37-N3-C40-C41	-81.2(12)
C38-N3-C40-C41	103.2(10)
C45-C40-C41-C42	-0.7(13)
N3-C40-C41-C42	-178.0(7)
C45-C40-C41-C46	176.9(9)
N3-C40-C41-C46	-0.5(12)
C40-C41-C42-C43	0.3(12)
C46-C41-C42-C43	-177.4(8)
C41-C42-C43-C44	0.0(13)
C42-C43-C44-C45	0.0(14)
C43-C44-C45-C40	-0.3(13)
C43-C44-C45-C49	178.4(8)
C41-C40-C45-C44	0.7(13)
N3-C40-C45-C44	178.0(8)
C41-C40-C45-C49	-178.0(8)
N3-C40-C45-C49	-0.7(12)
C42-C41-C46-C48	-59.8(13)
C40-C41-C46-C48	122.8(10)
C42-C41-C46-C47	61.5(12)
C40-C41-C46-C47	-116.0(11)
C44-C45-C49-C51	-71.6(11)
C40-C45-C49-C51	107.0(10)
C44-C45-C49-C50	51.6(12)
C40-C45-C49-C50	-129.8(10)

C37-N4-C52-C57	89.0(10)
C39-N4-C52-C57	-87.4(11)
C37-N4-C52-C53	-92.2(10)
C39-N4-C52-C53	91.4(10)
C57-C52-C53-C54	0.6(11)
N4-C52-C53-C54	-178.2(7)
C57-C52-C53-C58	-177.0(8)
N4-C52-C53-C58	4.2(11)
C52-C53-C54-C55	0.4(12)
C58-C53-C54-C55	178.1(8)
C53-C54-C55-C56	0.0(15)
C54-C55-C56-C57	-1.4(16)
C53-C52-C57-C56	-1.9(13)
N4-C52-C57-C56	176.8(8)
C53-C52-C57-C61	179.7(8)
N4-C52-C57-C61	-1.5(12)
C55-C56-C57-C52	2.3(15)
C55-C56-C57-C61	-179.4(10)
C54-C53-C58-C60	-73.7(11)
C52-C53-C58-C60	103.9(10)
C54-C53-C58-C59	51.9(11)
C52-C53-C58-C59	-130.5(9)
C52-C57-C61-C63	-118.3(10)
C56-C57-C61-C63	63.4(12)
C52-C57-C61-C62	121.5(10)
C56-C57-C61-C62	-56.8(13)
C1H-C2H-C3H-C4H	-174(6)
C2H-C3H-C4H-C5H	-168(6)
C1H'-C2H'-C3H'-C4H'	-176(4)
C2H'-C3H'-C4H'-C5H'	-176(4)

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (18b) CCDC 1572072.

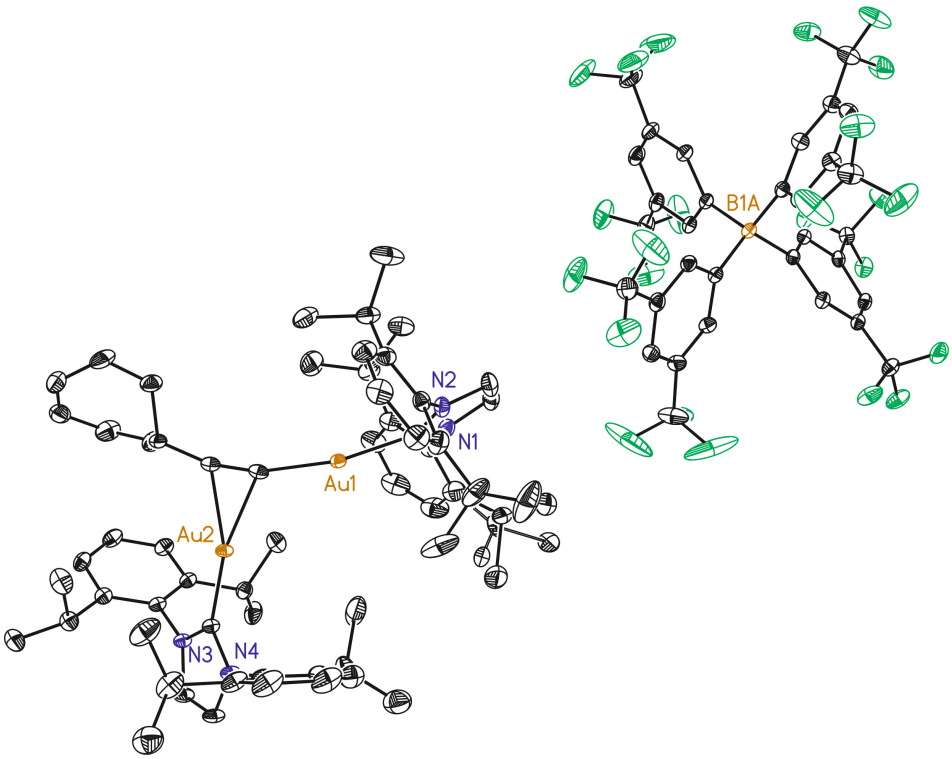


Table 1. Crystal data and structure refinement for sfc-a-141.

Identification code	sfc-a-141	
Empirical formula	C97.50 H97 Au2 B F24 N4	
Formula weight	2185.53	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.03400(10)Å	a= 83.8500(10)°.
	b = 16.07100(10)Å	b = 87.45°.
	c = 18.66030(10)Å	g = 78.5640(10)°.
Volume	4684.51(5) $Å^3$	
Z	2	
Density (calculated)	1.549 Mg/m^3	
Absorption coefficient	3.224 mm^{-1}	
F(000)	2178	
Crystal size	0.25 x 0.25 x 0.15 mm^3	
Theta range for data collection	2.196 to 37.386°.	
Index ranges	-27<=h<=27,-27<=k<=27,-31<=l<=31	
Reflections collected	226782	

Independent reflections	47268[R(int) = 0.0357]
Completeness to theta =37.386°	96.6%
Absorption correction	Multi-scan
Max. and min. transmission	0.643 and 0.495
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	47268/ 84/ 1217
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0258, wR2 = 0.0550
R indices (all data)	R1 = 0.0417, wR2 = 0.0586
Largest diff. peak and hole	1.732 and -1.144 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for sfc-a-141.

Bond lengths----

Au1-C63	1.9916(15)
Au1-C1	2.0120(15)
Au2-C28	1.9990(13)
Au2-C55	2.2034(14)
Au2-C63	2.2133(14)
N3-C28	1.3524(17)
N3-C29	1.3843(18)
N3-C31	1.4464(17)
N4-C28	1.3509(18)
N4-C30	1.3832(18)
N4-C43	1.4430(18)
N1-C1	1.3565(19)
N1-C2	1.383(2)
N1-C4	1.450(2)
N2-C1	1.351(2)
N2-C3	1.386(2)
N2-C16	1.440(2)
C2-C3	1.347(3)
C2-H2	0.9300
C3-H3	0.9300
C4-C9	1.396(2)
C4-C5	1.404(2)
C5-C6	1.392(2)
C5-C13	1.514(2)
C6-C7	1.380(3)

C6-H6	0.9300
C7-C8	1.365(3)
C7-H7	0.9300
C8-C9	1.413(3)
C8-H8	0.9300
C9-C10'	1.502(5)
C9-C10	1.522(4)
C10-C12	1.519(4)
C10-C11	1.579(4)
C10-H10	0.9800
C11-H11A	0.9600
C11-H11B	0.9600
C11-H11C	0.9600
C12-H12A	0.9600
C12-H12B	0.9600
C12-H12C	0.9600
C10'-C12'	1.512(5)
C10'-C11'	1.586(6)
C10'-H10'	0.9800
C11'-H11D	0.9600
C11'-H11E	0.9600
C11'-H11F	0.9600
C12'-H12D	0.9600
C12'-H12E	0.9600
C12'-H12F	0.9600
C13-C15	1.528(3)
C13-C14	1.536(3)
C13-H13	0.9800
C14-H14A	0.9600
C14-H14B	0.9600
C14-H14C	0.9600
C15-H15A	0.9600
C15-H15B	0.9600
C15-H15C	0.9600
C16-C21	1.397(2)
C16-C17	1.401(2)
C17-C18	1.395(2)
C17-C22	1.518(3)

C18-C19	1.378(3)
C18-H18	0.9300
C19-C20	1.384(3)
C19-H19	0.9300
C20-C21	1.395(2)
C20-H20	0.9300
C21-C25	1.514(2)
C22-C24	1.526(4)
C22-C23	1.533(3)
C22-H22	0.9800
C23-H23A	0.9600
C23-H23B	0.9600
C23-H23C	0.9600
C24-H24A	0.9600
C24-H24B	0.9600
C24-H24C	0.9600
C25-C26	1.530(2)
C25-C27	1.533(3)
C25-H25	0.9800
C26-H26A	0.9600
C26-H26B	0.9600
C26-H26C	0.9600
C27-H27A	0.9600
C27-H27B	0.9600
C27-H27C	0.9600
C29-C30	1.350(2)
C29-H29	0.9300
C30-H30	0.9300
C31-C32	1.399(2)
C31-C36	1.402(2)
C32-C33	1.394(2)
C32-C37	1.515(2)
C33-C34	1.385(2)
C33-H33	0.9300
C34-C35	1.385(2)
C34-H34	0.9300
C35-C36	1.396(2)
C35-H35	0.9300

C36-C40	1.517(2)
C37-C39	1.527(2)
C37-C38	1.528(2)
C37-H37	0.9800
C38-H38A	0.9600
C38-H38B	0.9600
C38-H38C	0.9600
C39-H39A	0.9600
C39-H39B	0.9600
C39-H39C	0.9600
C40-C42	1.531(2)
C40-C41	1.534(2)
C40-H40	0.9800
C41-H41A	0.9600
C41-H41B	0.9600
C41-H41C	0.9600
C42-H42A	0.9600
C42-H42B	0.9600
C42-H42C	0.9600
C43-C48	1.394(2)
C43-C44	1.396(2)
C44-C45	1.399(2)
C44-C49	1.515(3)
C45-C46	1.377(3)
C45-H45	0.9300
C46-C47	1.382(3)
C46-H46	0.9300
C47-C48	1.398(2)
C47-H47	0.9300
C48-C52	1.517(3)
C49-C50	1.534(3)
C49-C51	1.534(3)
C49-H49	0.9800
C50-H50A	0.9600
C50-H50B	0.9600
C50-H50C	0.9600
C51-H51A	0.9600
C51-H51B	0.9600

C51-H51C	0.9600
C52-C54	1.521(3)
C52-C53	1.531(3)
C52-H52	0.9800
C53-H53A	0.9600
C53-H53B	0.9600
C53-H53C	0.9600
C54-H54A	0.9600
C54-H54B	0.9600
C54-H54C	0.9600
C55-C63	1.231(2)
C55-C56	1.478(2)
C56-C62	1.504(2)
C56-C57	1.507(2)
C56-H56	0.9800
C57-C58	1.340(2)
C57-H57	0.9300
C58-C59	1.444(3)
C58-H58	0.9300
C59-C60	1.344(3)
C59-H59	0.9300
C60-C61	1.436(3)
C60-H60	0.9300
C61-C62	1.338(3)
C61-H61	0.9300
C62-H62	0.9300
B1A-C1A	1.637(2)
B1A-C17A	1.637(2)
B1A-C9A	1.646(2)
B1A-C25A	1.647(2)
C1A-C2A	1.397(2)
C1A-C6A	1.4037(19)
C2A-C3A	1.392(2)
C2A-H2A	0.9300
C3A-C4A	1.386(2)
C3A-C7A	1.490(2)
C4A-C5A	1.389(2)
C4A-H4A	0.9300

C5A-C6A	1.392(2)
C5A-C8A	1.498(2)
C6A-H6A	0.9300
C7A-F3A	1.316(2)
C7A-F1A	1.317(3)
C7A-F2A	1.333(3)
C8A-F6A	1.316(2)
C8A-F5A	1.331(2)
C8A-F4A	1.337(2)
C9A-C14A	1.399(2)
C9A-C10A	1.401(2)
C10A-C11A	1.391(2)
C10A-H10A	0.9300
C11A-C12A	1.388(2)
C11A-C15A	1.495(2)
C12A-C13A	1.388(2)
C12A-H12X	0.9300
C13A-C14A	1.393(2)
C13A-C16A	1.497(2)
C14A-H14D	0.9300
C15A-F8A	1.329(2)
C15A-F9A	1.3294(19)
C15A-F7A	1.330(2)
C16A-F12A	1.333(3)
C16A-F11A	1.339(3)
C16A-F10A	1.340(2)
C17A-C18A	1.400(2)
C17A-C22A	1.4078(19)
C18A-C19A	1.389(2)
C18A-H18A	0.9300
C19A-C20A	1.384(2)
C19A-C23A	1.490(2)
C20A-C21A	1.391(2)
C20A-H20A	0.9300
C21A-C22A	1.391(2)
C21A-C24A	1.500(2)
C22A-H22A	0.9300
C23A-F15A	1.3388(19)

C23A-F13A	1.342(2)
C23A-F14A	1.352(2)
C24A-F17A	1.326(2)
C24A-F16A	1.334(2)
C24A-F18A	1.337(2)
C25A-C26A	1.3969(19)
C25A-C30A	1.4022(19)
C26A-C27A	1.3961(19)
C26A-H26D	0.9300
C27A-C28A	1.387(2)
C27A-C31A	1.493(2)
C28A-C29A	1.3910(19)
C28A-H28A	0.9300
C29A-C30A	1.3942(19)
C29A-C32A	1.497(2)
C30A-H30A	0.9300
C31A-F24A	1.3440(17)
C31A-F22A	1.3443(18)
C31A-F23A	1.3479(17)
C32A-F20A	1.3357(17)
C32A-F21A	1.3405(18)
C32A-F19A	1.3421(18)
C1S-C2S	1.5673
C1S-H1S1	0.9600
C1S-H1S2	0.9600
C1S-H1S3	0.9600
C2S-C3S	1.5017
C2S-H2S1	0.9700
C2S-H2S2	0.9700
C3S-C4S	1.5523
C3S-H3S1	0.9700
C3S-H3S2	0.9700
C4S-C5S	1.4803
C4S-H4S1	0.9700
C4S-H4S2	0.9700
C5S-H5S1	0.9600
C5S-H5S2	0.9600
C5S-H5S3	0.9600

Angles----------

C63-Au1-C1	167.87(6)
C28-Au2-C55	159.90(6)
C28-Au2-C63	167.39(6)
C55-Au2-C63	32.35(6)
C28-N3-C29	110.62(11)
C28-N3-C31	123.99(11)
C29-N3-C31	125.34(11)
C28-N4-C30	110.91(12)
C28-N4-C43	123.57(12)
C30-N4-C43	125.40(12)
C1-N1-C2	110.78(14)
C1-N1-C4	122.41(13)
C2-N1-C4	126.59(13)
C1-N2-C3	110.87(14)
C1-N2-C16	123.51(12)
C3-N2-C16	125.61(14)
N2-C1-N1	104.84(13)
N2-C1-Au1	126.92(11)
N1-C1-Au1	126.58(11)
C3-C2-N1	106.79(14)
C3-C2-H2	126.6
N1-C2-H2	126.6
C2-C3-N2	106.71(15)
C2-C3-H3	126.6
N2-C3-H3	126.6
C9-C4-C5	123.07(17)
C9-C4-N1	119.15(16)
C5-C4-N1	117.74(14)
C6-C5-C4	117.69(17)
C6-C5-C13	120.66(17)
C4-C5-C13	121.51(15)
C7-C6-C5	120.5(2)
C7-C6-H6	119.8
C5-C6-H6	119.8
C8-C7-C6	120.9(2)
C8-C7-H7	119.6

C6-C7-H7	119.6
C7-C8-C9	121.56(19)
C7-C8-H8	119.2
C9-C8-H8	119.2
C4-C9-C8	116.21(19)
C4-C9-C10'	128.7(5)
C8-C9-C10'	114.9(6)
C4-C9-C10	121.4(2)
C8-C9-C10	122.2(2)
C12-C10-C9	106.6(2)
C12-C10-C11	106.6(2)
C9-C10-C11	109.9(2)
C12-C10-H10	111.2
C9-C10-H10	111.2
C11-C10-H10	111.2
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5
C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C9-C10'-C12'	135.6(8)
C9-C10'-C11'	117.8(7)
C12'-C10'-C11'	106.6(6)
C9-C10'-H10'	90.4
C12'-C10'-H10'	90.4
C11'-C10'-H10'	90.4
C10'-C11'-H11D	109.5
C10'-C11'-H11E	109.5
H11D-C11'-H11E	109.5
C10'-C11'-H11F	109.5
H11D-C11'-H11F	109.5

H11E-C11'-H11F	109.5
C10'-C12'-H12D	109.5
C10'-C12'-H12E	109.5
H12D-C12'-H12E	109.5
C10'-C12'-H12F	109.5
H12D-C12'-H12F	109.5
H12E-C12'-H12F	109.5
C5-C13-C15	113.40(16)
C5-C13-C14	109.94(15)
C15-C13-C14	111.22(15)
C5-C13-H13	107.3
C15-C13-H13	107.3
C14-C13-H13	107.3
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C21-C16-C17	123.87(15)
C21-C16-N2	118.60(13)
C17-C16-N2	117.51(14)
C18-C17-C16	116.78(16)
C18-C17-C22	121.27(15)
C16-C17-C22	121.89(15)
C19-C18-C17	120.95(16)
C19-C18-H18	119.5
C17-C18-H18	119.5
C18-C19-C20	120.72(17)
C18-C19-H19	119.6
C20-C19-H19	119.6
C19-C20-C21	121.13(17)

C19-C20-H20	119.4
C21-C20-H20	119.4
C20-C21-C16	116.55(15)
C20-C21-C25	121.03(15)
C16-C21-C25	122.41(15)
C17-C22-C24	110.47(18)
C17-C22-C23	111.8(2)
C24-C22-C23	112.8(2)
C17-C22-H22	107.2
C24-C22-H22	107.2
C23-C22-H22	107.2
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C21-C25-C26	111.70(14)
C21-C25-C27	111.35(15)
C26-C25-C27	110.97(16)
C21-C25-H25	107.5
C26-C25-H25	107.5
C27-C25-H25	107.5
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5

C25-C27-H27C	109.5
H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
N4-C28-N3	105.07(11)
N4-C28-Au2	128.00(10)
N3-C28-Au2	126.88(10)
C30-C29-N3	106.85(12)
C30-C29-H29	126.6
N3-C29-H29	126.6
C29-C30-N4	106.55(12)
C29-C30-H30	126.7
N4-C30-H30	126.7
C32-C31-C36	123.46(13)
C32-C31-N3	118.05(12)
C36-C31-N3	118.49(13)
C33-C32-C31	117.38(13)
C33-C32-C37	119.59(13)
C31-C32-C37	123.03(12)
C34-C33-C32	120.59(14)
C34-C33-H33	119.7
C32-C33-H33	119.7
C35-C34-C33	120.70(14)
C35-C34-H34	119.7
C33-C34-H34	119.7
C34-C35-C36	121.17(14)
C34-C35-H35	119.4
C36-C35-H35	119.4
C35-C36-C31	116.69(13)
C35-C36-C40	120.75(14)
C31-C36-C40	122.49(13)
C32-C37-C39	110.57(13)
C32-C37-C38	111.72(13)
C39-C37-C38	110.24(14)
C32-C37-H37	108.1
C39-C37-H37	108.1
C38-C37-H37	108.1
C37-C38-H38A	109.5
C37-C38-H38B	109.5

H38A-C38-H38B	109.5
C37-C38-H38C	109.5
H38A-C38-H38C	109.5
H38B-C38-H38C	109.5
C37-C39-H39A	109.5
C37-C39-H39B	109.5
H39A-C39-H39B	109.5
C37-C39-H39C	109.5
H39A-C39-H39C	109.5
H39B-C39-H39C	109.5
C36-C40-C42	112.51(13)
C36-C40-C41	109.95(13)
C42-C40-C41	110.51(14)
C36-C40-H40	107.9
C42-C40-H40	107.9
C41-C40-H40	107.9
C40-C41-H41A	109.5
C40-C41-H41B	109.5
H41A-C41-H41B	109.5
C40-C41-H41C	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
C40-C42-H42A	109.5
C40-C42-H42B	109.5
H42A-C42-H42B	109.5
C40-C42-H42C	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
C48-C43-C44	124.24(14)
C48-C43-N4	117.40(15)
C44-C43-N4	118.35(14)
C43-C44-C45	116.44(17)
C43-C44-C49	121.73(14)
C45-C44-C49	121.80(17)
C46-C45-C44	120.98(19)
C46-C45-H45	119.5
C44-C45-H45	119.5
C45-C46-C47	120.93(16)

C45-C46-H46	119.5
C47-C46-H46	119.5
C46-C47-C48	120.79(18)
C46-C47-H47	119.6
C48-C47-H47	119.6
C43-C48-C47	116.58(18)
C43-C48-C52	122.95(14)
C47-C48-C52	120.46(17)
C44-C49-C50	113.20(17)
C44-C49-C51	110.65(19)
C50-C49-C51	110.03(17)
C44-C49-H49	107.6
C50-C49-H49	107.6
C51-C49-H49	107.6
C49-C50-H50A	109.5
C49-C50-H50B	109.5
H50A-C50-H50B	109.5
C49-C50-H50C	109.5
H50A-C50-H50C	109.5
H50B-C50-H50C	109.5
C49-C51-H51A	109.5
C49-C51-H51B	109.5
H51A-C51-H51B	109.5
C49-C51-H51C	109.5
H51A-C51-H51C	109.5
H51B-C51-H51C	109.5
C48-C52-C54	111.90(17)
C48-C52-C53	111.18(19)
C54-C52-C53	110.56(17)
C48-C52-H52	107.7
C54-C52-H52	107.7
C53-C52-H52	107.7
C52-C53-H53A	109.5
C52-C53-H53B	109.5
H53A-C53-H53B	109.5
C52-C53-H53C	109.5
H53A-C53-H53C	109.5
H53B-C53-H53C	109.5

C52-C54-H54A	109.5
C52-C54-H54B	109.5
H54A-C54-H54B	109.5
C52-C54-H54C	109.5
H54A-C54-H54C	109.5
H54B-C54-H54C	109.5
C63-C55-C56	165.46(15)
C63-C55-Au2	74.27(9)
C56-C55-Au2	118.90(10)
C55-C56-C62	111.56(13)
C55-C56-C57	112.08(13)
C62-C56-C57	107.02(13)
C55-C56-H56	108.7
C62-C56-H56	108.7
C57-C56-H56	108.7
C58-C57-C56	119.95(15)
C58-C57-H57	120.0
C56-C57-H57	120.0
C57-C58-C59	125.17(16)
C57-C58-H58	117.4
C59-C58-H58	117.4
C60-C59-C58	125.22(18)
C60-C59-H59	117.4
C58-C59-H59	117.4
C59-C60-C61	125.92(17)
C59-C60-H60	117.0
C61-C60-H60	117.0
C62-C61-C60	124.60(18)
C62-C61-H61	117.7
C60-C61-H61	117.7
C61-C62-C56	121.24(17)
C61-C62-H62	119.4
C56-C62-H62	119.4
C55-C63-Au1	162.80(12)
C55-C63-Au2	73.38(9)
Au1-C63-Au2	121.47(7)
C1A-B1A-C17A	112.99(11)
C1A-B1A-C9A	105.67(11)

C17A-B1A-C9A	112.47(11)
C1A-B1A-C25A	111.74(11)
C17A-B1A-C25A	104.84(11)
C9A-B1A-C25A	109.20(11)
C2A-C1A-C6A	115.85(13)
C2A-C1A-B1A	121.82(12)
C6A-C1A-B1A	122.14(12)
C3A-C2A-C1A	122.17(13)
C3A-C2A-H2A	118.9
C1A-C2A-H2A	118.9
C4A-C3A-C2A	121.02(14)
C4A-C3A-C7A	119.28(14)
C2A-C3A-C7A	119.59(14)
C3A-C4A-C5A	117.99(13)
C3A-C4A-H4A	121.0
C5A-C4A-H4A	121.0
C4A-C5A-C6A	120.73(13)
C4A-C5A-C8A	118.76(14)
C6A-C5A-C8A	120.51(14)
C5A-C6A-C1A	122.20(13)
C5A-C6A-H6A	118.9
C1A-C6A-H6A	118.9
F3A-C7A-F1A	107.0(2)
F3A-C7A-F2A	105.77(18)
F1A-C7A-F2A	105.2(2)
F3A-C7A-C3A	114.72(15)
F1A-C7A-C3A	111.96(18)
F2A-C7A-C3A	111.57(18)
F6A-C8A-F5A	107.40(17)
F6A-C8A-F4A	106.85(17)
F5A-C8A-F4A	104.64(14)
F6A-C8A-C5A	113.12(14)
F5A-C8A-C5A	112.04(15)
F4A-C8A-C5A	112.25(14)
C14A-C9A-C10A	115.53(13)
C14A-C9A-B1A	124.40(12)
C10A-C9A-B1A	120.06(12)
C11A-C10A-C9A	122.89(14)

C11A-C10A-H10A	118.6
C9A-C10A-H10A	118.6
C12A-C11A-C10A	120.53(15)
C12A-C11A-C15A	119.55(14)
C10A-C11A-C15A	119.77(14)
C13A-C12A-C11A	117.65(14)
C13A-C12A-H12X	121.2
C11A-C12A-H12X	121.2
C12A-C13A-C14A	121.54(14)
C12A-C13A-C16A	118.39(15)
C14A-C13A-C16A	119.96(16)
C13A-C14A-C9A	121.81(14)
C13A-C14A-H14D	119.1
C9A-C14A-H14D	119.1
F8A-C15A-F9A	105.98(15)
F8A-C15A-F7A	106.46(17)
F9A-C15A-F7A	105.56(16)
F8A-C15A-C11A	111.78(16)
F9A-C15A-C11A	113.42(15)
F7A-C15A-C11A	113.06(15)
F12A-C16A-F11A	105.41(19)
F12A-C16A-F10A	105.89(17)
F11A-C16A-F10A	106.89(17)
F12A-C16A-C13A	113.50(16)
F11A-C16A-C13A	111.89(17)
F10A-C16A-C13A	112.71(18)
C18A-C17A-C22A	115.28(13)
C18A-C17A-B1A	119.66(12)
C22A-C17A-B1A	124.87(12)
C19A-C18A-C17A	122.66(13)
C19A-C18A-H18A	118.7
C17A-C18A-H18A	118.7
C20A-C19A-C18A	121.20(13)
C20A-C19A-C23A	121.20(14)
C18A-C19A-C23A	117.59(13)
C19A-C20A-C21A	117.46(14)
C19A-C20A-H20A	121.3
C21A-C20A-H20A	121.3

C22A-C21A-C20A	121.31(13)
C22A-C21A-C24A	120.09(14)
C20A-C21A-C24A	118.59(14)
C21A-C22A-C17A	122.04(13)
C21A-C22A-H22A	119.0
C17A-C22A-H22A	119.0
F15A-C23A-F13A	106.88(14)
F15A-C23A-F14A	106.36(14)
F13A-C23A-F14A	105.25(13)
F15A-C23A-C19A	113.50(13)
F13A-C23A-C19A	112.44(14)
F14A-C23A-C19A	111.85(14)
F17A-C24A-F16A	106.61(16)
F17A-C24A-F18A	105.90(16)
F16A-C24A-F18A	105.49(15)
F17A-C24A-C21A	113.15(14)
F16A-C24A-C21A	112.70(14)
F18A-C24A-C21A	112.40(15)
C26A-C25A-C30A	115.64(12)
C26A-C25A-B1A	121.67(12)
C30A-C25A-B1A	122.64(12)
C27A-C26A-C25A	122.30(13)
C27A-C26A-H26D	118.8
C25A-C26A-H26D	118.8
C28A-C27A-C26A	121.00(13)
C28A-C27A-C31A	119.99(12)
C26A-C27A-C31A	119.00(13)
C27A-C28A-C29A	117.71(12)
C27A-C28A-H28A	121.1
C29A-C28A-H28A	121.1
C28A-C29A-C30A	120.90(13)
C28A-C29A-C32A	118.34(12)
C30A-C29A-C32A	120.71(13)
C29A-C30A-C25A	122.26(13)
C29A-C30A-H30A	118.9
C25A-C30A-H30A	118.9
F24A-C31A-F22A	106.28(12)
F24A-C31A-F23A	106.34(11)

F22A-C31A-F23A	106.16(12)
F24A-C31A-C27A	112.80(12)
F22A-C31A-C27A	112.27(12)
F23A-C31A-C27A	112.49(12)
F20A-C32A-F21A	106.63(13)
F20A-C32A-F19A	106.10(12)
F21A-C32A-F19A	105.97(13)
F20A-C32A-C29A	113.04(12)
F21A-C32A-C29A	112.86(12)
F19A-C32A-C29A	111.71(13)
C2S-C1S-H1S1	109.5
C2S-C1S-H1S2	109.5
H1S1-C1S-H1S2	109.5
C2S-C1S-H1S3	109.5
H1S1-C1S-H1S3	109.5
H1S2-C1S-H1S3	109.5
C3S-C2S-C1S	113.3
C3S-C2S-H2S1	108.9
C1S-C2S-H2S1	108.9
C3S-C2S-H2S2	108.9
C1S-C2S-H2S2	108.9
H2S1-C2S-H2S2	107.7
C2S-C3S-C4S	112.9
C2S-C3S-H3S1	109.0
C4S-C3S-H3S1	109.0
C2S-C3S-H3S2	109.0
C4S-C3S-H3S2	109.0
H3S1-C3S-H3S2	107.8
C5S-C4S-C3S	116.7
C5S-C4S-H4S1	108.1
C3S-C4S-H4S1	108.1
C5S-C4S-H4S2	108.1
C3S-C4S-H4S2	108.1
H4S1-C4S-H4S2	107.3
C4S-C5S-H5S1	109.5
C4S-C5S-H5S2	109.5
H5S1-C5S-H5S2	109.5
C4S-C5S-H5S3	109.5

H5S1-C5S-H5S3	109.5
H5S2-C5S-H5S3	109.5

Table 3. Torsion angles [°] for sfc-a-141.

C3-N2-C1-N1	-0.11(17)
C16-N2-C1-N1	178.90(13)
C3-N2-C1-Au1	-166.10(11)
C16-N2-C1-Au1	12.9(2)
C2-N1-C1-N2	-0.23(17)
C4-N1-C1-N2	-175.09(13)
C2-N1-C1-Au1	165.83(11)
C4-N1-C1-Au1	-9.0(2)
C1-N1-C2-C3	0.48(19)
C4-N1-C2-C3	175.08(15)
N1-C2-C3-N2	-0.52(19)
C1-N2-C3-C2	0.40(19)
C16-N2-C3-C2	-178.57(15)
C1-N1-C4-C9	-106.50(18)
C2-N1-C4-C9	79.5(2)
C1-N1-C4-C5	71.4(2)
C2-N1-C4-C5	-102.64(19)
C9-C4-C5-C6	2.8(3)
N1-C4-C5-C6	-174.99(15)
C9-C4-C5-C13	-173.06(16)
N1-C4-C5-C13	9.2(2)
C4-C5-C6-C7	-1.3(3)
C13-C5-C6-C7	174.60(17)
C5-C6-C7-C8	-1.4(3)
C6-C7-C8-C9	2.8(3)
C5-C4-C9-C8	-1.5(3)
N1-C4-C9-C8	176.24(15)
C5-C4-C9-C10'	-175.1(6)
N1-C4-C9-C10'	2.6(6)
C5-C4-C9-C10	172.87(19)
N1-C4-C9-C10	-9.4(3)
C7-C8-C9-C4	-1.3(3)
C7-C8-C9-C10'	173.2(5)

C7-C8-C9-C10	-175.6(2)
C4-C9-C10-C12	-110.1(3)
C8-C9-C10-C12	63.9(3)
C4-C9-C10-C11	134.8(2)
C8-C9-C10-C11	-51.2(3)
C4-C9-C10'-C12'	-122.0(14)
C8-C9-C10'-C12'	64.3(17)
C4-C9-C10'-C11'	59.7(13)
C8-C9-C10'-C11'	-114.0(10)
C6-C5-C13-C15	37.0(2)
C4-C5-C13-C15	-147.28(17)
C6-C5-C13-C14	-88.2(2)
C4-C5-C13-C14	87.50(19)
C1-N2-C16-C21	-87.89(19)
C3-N2-C16-C21	90.96(19)
C1-N2-C16-C17	90.95(18)
C3-N2-C16-C17	-90.2(2)
C21-C16-C17-C18	-0.2(3)
N2-C16-C17-C18	-179.01(15)
C21-C16-C17-C22	176.88(17)
N2-C16-C17-C22	-1.9(2)
C16-C17-C18-C19	-0.4(3)
C22-C17-C18-C19	-177.49(19)
C17-C18-C19-C20	0.5(3)
C18-C19-C20-C21	-0.1(3)
C19-C20-C21-C16	-0.5(3)
C19-C20-C21-C25	178.50(17)
C17-C16-C21-C20	0.6(2)
N2-C16-C21-C20	179.41(14)
C17-C16-C21-C25	-178.33(16)
N2-C16-C21-C25	0.4(2)
C18-C17-C22-C24	75.1(2)
C16-C17-C22-C24	-101.8(2)
C18-C17-C22-C23	-51.3(3)
C16-C17-C22-C23	131.7(2)
C20-C21-C25-C26	63.0(2)
C16-C21-C25-C26	-118.04(19)
C20-C21-C25-C27	-61.6(2)

C16-C21-C25-C27	117.28(18)
C30-N4-C28-N3	-0.30(17)
C43-N4-C28-N3	-176.51(14)
C30-N4-C28-Au2	-177.69(11)
C43-N4-C28-Au2	6.1(2)
C29-N3-C28-N4	0.23(16)
C31-N3-C28-N4	-177.23(13)
C29-N3-C28-Au2	177.65(11)
C31-N3-C28-Au2	0.2(2)
C28-N3-C29-C30	-0.07(18)
C31-N3-C29-C30	177.35(14)
N3-C29-C30-N4	-0.11(18)
C28-N4-C30-C29	0.26(19)
C43-N4-C30-C29	176.39(15)
C28-N3-C31-C32	81.05(17)
C29-N3-C31-C32	-96.03(17)
C28-N3-C31-C36	-99.04(17)
C29-N3-C31-C36	83.87(18)
C36-C31-C32-C33	0.6(2)
N3-C31-C32-C33	-179.51(12)
C36-C31-C32-C37	-178.64(13)
N3-C31-C32-C37	1.3(2)
C31-C32-C33-C34	-1.1(2)
C37-C32-C33-C34	178.10(14)
C32-C33-C34-C35	0.9(2)
C33-C34-C35-C36	0.1(2)
C34-C35-C36-C31	-0.6(2)
C34-C35-C36-C40	176.37(14)
C32-C31-C36-C35	0.3(2)
N3-C31-C36-C35	-179.62(12)
C32-C31-C36-C40	-176.65(13)
N3-C31-C36-C40	3.5(2)
C33-C32-C37-C39	-61.49(19)
C31-C32-C37-C39	117.72(16)
C33-C32-C37-C38	61.69(18)
C31-C32-C37-C38	-119.10(16)
C35-C36-C40-C42	43.6(2)
C31-C36-C40-C42	-139.61(15)

C35-C36-C40-C41	-80.05(18)
C31-C36-C40-C41	96.76(17)
C28-N4-C43-C48	85.28(19)
C30-N4-C43-C48	-90.38(19)
C28-N4-C43-C44	-94.47(18)
C30-N4-C43-C44	89.87(19)
C48-C43-C44-C45	-2.1(2)
N4-C43-C44-C45	177.62(14)
C48-C43-C44-C49	179.71(17)
N4-C43-C44-C49	-0.6(2)
C43-C44-C45-C46	0.3(3)
C49-C44-C45-C46	178.50(18)
C44-C45-C46-C47	1.2(3)
C45-C46-C47-C48	-1.1(3)
C44-C43-C48-C47	2.2(2)
N4-C43-C48-C47	-177.52(15)
C44-C43-C48-C52	-178.44(16)
N4-C43-C48-C52	1.8(2)
C46-C47-C48-C43	-0.5(3)
C46-C47-C48-C52	-179.89(18)
C43-C44-C49-C50	-143.84(18)
C45-C44-C49-C50	38.1(3)
C43-C44-C49-C51	92.1(2)
C45-C44-C49-C51	-86.0(2)
C43-C48-C52-C54	122.63(19)
C47-C48-C52-C54	-58.0(2)
C43-C48-C52-C53	-113.21(19)
C47-C48-C52-C53	66.1(2)
C63-C55-C56-C62	84.3(6)
Au2-C55-C56-C62	-69.21(15)
C63-C55-C56-C57	-35.7(7)
Au2-C55-C56-C57	170.79(11)
C55-C56-C57-C58	-168.00(17)
C62-C56-C57-C58	69.4(2)
C56-C57-C58-C59	-8.3(3)
C57-C58-C59-C60	-34.0(3)
C58-C59-C60-C61	1.6(3)
C59-C60-C61-C62	33.0(3)

C60-C61-C62-C56	6.1(3)
C55-C56-C62-C61	169.00(17)
C57-C56-C62-C61	-68.1(2)
C56-C55-C63-Au1	-4.6(10)
Au2-C55-C63-Au1	151.4(4)
C56-C55-C63-Au2	-156.0(6)
C17A-B1A-C1A-C2A	-147.25(13)
C9A-B1A-C1A-C2A	89.37(15)
C25A-B1A-C1A-C2A	-29.30(17)
C17A-B1A-C1A-C6A	37.96(17)
C9A-B1A-C1A-C6A	-85.42(15)
C25A-B1A-C1A-C6A	155.91(12)
C6A-C1A-C2A-C3A	-1.9(2)
B1A-C1A-C2A-C3A	-176.99(13)
C1A-C2A-C3A-C4A	0.2(2)
C1A-C2A-C3A-C7A	-175.89(16)
C2A-C3A-C4A-C5A	1.1(2)
C7A-C3A-C4A-C5A	177.18(16)
C3A-C4A-C5A-C6A	-0.6(2)
C3A-C4A-C5A-C8A	178.69(15)
C4A-C5A-C6A-C1A	-1.2(2)
C8A-C5A-C6A-C1A	179.51(14)
C2A-C1A-C6A-C5A	2.4(2)
B1A-C1A-C6A-C5A	177.49(13)
C4A-C3A-C7A-F3A	152.50(18)
C2A-C3A-C7A-F3A	-31.3(3)
C4A-C3A-C7A-F1A	30.4(3)
C2A-C3A-C7A-F1A	-153.5(2)
C4A-C3A-C7A-F2A	-87.3(2)
C2A-C3A-C7A-F2A	88.9(2)
C4A-C5A-C8A-F6A	155.75(17)
C6A-C5A-C8A-F6A	-25.0(2)
C4A-C5A-C8A-F5A	-82.67(19)
C6A-C5A-C8A-F5A	96.60(19)
C4A-C5A-C8A-F4A	34.7(2)
C6A-C5A-C8A-F4A	-146.00(16)
C1A-B1A-C9A-C14A	100.58(15)
C17A-B1A-C9A-C14A	-23.13(19)

C25A-B1A-C9A-C14A	-139.08(14)
C1A-B1A-C9A-C10A	-78.14(15)
C17A-B1A-C9A-C10A	158.15(12)
C25A-B1A-C9A-C10A	42.20(17)
C14A-C9A-C10A-C11A	2.9(2)
B1A-C9A-C10A-C11A	-178.25(13)
C9A-C10A-C11A-C12A	-2.1(2)
C9A-C10A-C11A-C15A	173.45(15)
C10A-C11A-C12A-C13A	0.2(2)
C15A-C11A-C12A-C13A	-175.39(16)
C11A-C12A-C13A-C14A	0.7(3)
C11A-C12A-C13A-C16A	176.96(16)
C12A-C13A-C14A-C9A	0.2(3)
C16A-C13A-C14A-C9A	-175.93(16)
C10A-C9A-C14A-C13A	-2.0(2)
B1A-C9A-C14A-C13A	179.24(14)
C12A-C11A-C15A-F8A	89.4(2)
C10A-C11A-C15A-F8A	-86.1(2)
C12A-C11A-C15A-F9A	-30.3(2)
C10A-C11A-C15A-F9A	154.12(16)
C12A-C11A-C15A-F7A	-150.43(17)
C10A-C11A-C15A-F7A	34.0(2)
C12A-C13A-C16A-F12A	161.27(17)
C14A-C13A-C16A-F12A	-22.4(3)
C12A-C13A-C16A-F11A	-79.6(2)
C14A-C13A-C16A-F11A	96.7(2)
C12A-C13A-C16A-F10A	40.9(3)
C14A-C13A-C16A-F10A	-142.80(18)
C1A-B1A-C17A-C18A	-162.18(12)
C9A-B1A-C17A-C18A	-42.64(17)
C25A-B1A-C17A-C18A	75.91(15)
C1A-B1A-C17A-C22A	23.04(18)
C9A-B1A-C17A-C22A	142.58(13)
C25A-B1A-C17A-C22A	-98.88(15)
C22A-C17A-C18A-C19A	-1.6(2)
B1A-C17A-C18A-C19A	-176.86(13)
C17A-C18A-C19A-C20A	0.1(2)
C17A-C18A-C19A-C23A	179.46(14)

C18A-C19A-C20A-C21A	0.7(2)
C23A-C19A-C20A-C21A	-178.66(15)
C19A-C20A-C21A-C22A	0.1(2)
C19A-C20A-C21A-C24A	179.14(15)
C20A-C21A-C22A-C17A	-1.7(2)
C24A-C21A-C22A-C17A	179.26(14)
C18A-C17A-C22A-C21A	2.4(2)
B1A-C17A-C22A-C21A	177.38(13)
C20A-C19A-C23A-F15A	-7.3(2)
C18A-C19A-C23A-F15A	173.30(15)
C20A-C19A-C23A-F13A	-128.81(16)
C18A-C19A-C23A-F13A	51.8(2)
C20A-C19A-C23A-F14A	113.01(17)
C18A-C19A-C23A-F14A	-66.35(19)
C22A-C21A-C24A-F17A	-29.0(2)
C20A-C21A-C24A-F17A	152.00(17)
C22A-C21A-C24A-F16A	-150.01(16)
C20A-C21A-C24A-F16A	31.0(2)
C22A-C21A-C24A-F18A	90.94(19)
C20A-C21A-C24A-F18A	-88.10(19)
C1A-B1A-C25A-C26A	144.37(13)
C17A-B1A-C25A-C26A	-92.90(14)
C9A-B1A-C25A-C26A	27.82(17)
C1A-B1A-C25A-C30A	-38.34(17)
C17A-B1A-C25A-C30A	84.38(15)
C9A-B1A-C25A-C30A	-154.89(13)
C30A-C25A-C26A-C27A	4.5(2)
B1A-C25A-C26A-C27A	-178.04(12)
C25A-C26A-C27A-C28A	-1.4(2)
C25A-C26A-C27A-C31A	179.57(13)
C26A-C27A-C28A-C29A	-2.4(2)
C31A-C27A-C28A-C29A	176.55(13)
C27A-C28A-C29A-C30A	3.0(2)
C27A-C28A-C29A-C32A	-174.61(13)
C28A-C29A-C30A-C25A	0.2(2)
C32A-C29A-C30A-C25A	177.78(13)
C26A-C25A-C30A-C29A	-3.9(2)
B1A-C25A-C30A-C29A	178.68(13)

C28A-C27A-C31A-F24A	23.69(18)
C26A-C27A-C31A-F24A	-157.30(12)
C28A-C27A-C31A-F22A	-96.35(16)
C26A-C27A-C31A-F22A	82.65(16)
C28A-C27A-C31A-F23A	143.98(13)
C26A-C27A-C31A-F23A	-37.02(18)
C28A-C29A-C32A-F20A	-38.01(19)
C30A-C29A-C32A-F20A	144.34(14)
C28A-C29A-C32A-F21A	-159.13(13)
C30A-C29A-C32A-F21A	23.2(2)
C28A-C29A-C32A-F19A	81.57(17)
C30A-C29A-C32A-F19A	-96.08(17)
C1S-C2S-C3S-C4S	179.6
C2S-C3S-C4S-C5S	-179.1

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)]gold (13) CCDC 1572070.

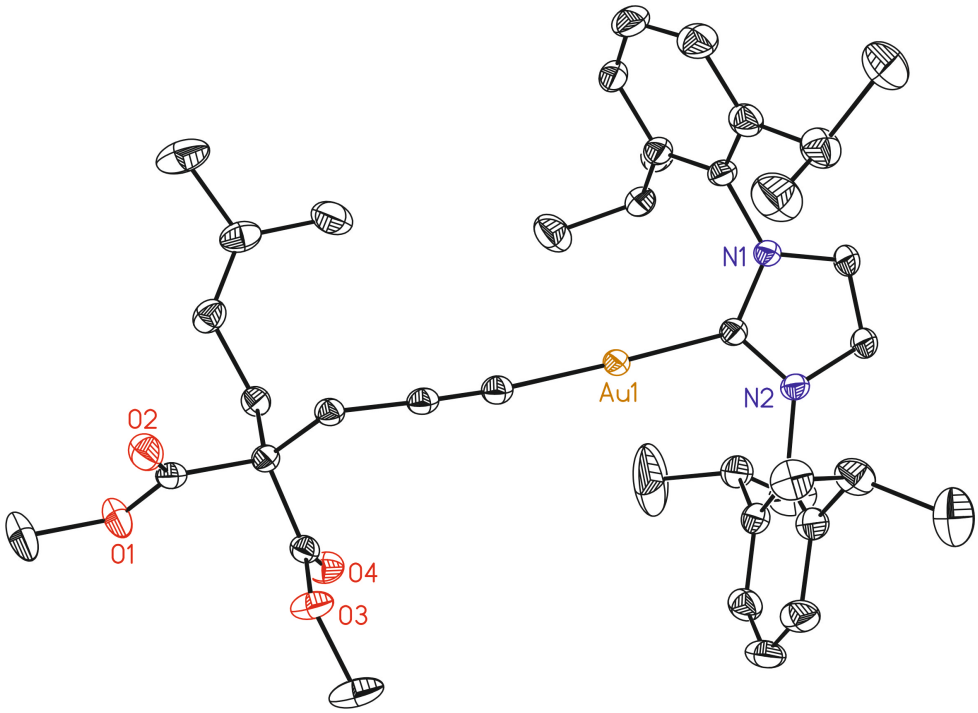


Table 1. Crystal data and structure refinement for SFC-A1.

Identification code	SFC-A1
Empirical formula	C45 H65 Au N2 O4

Formula weight	894.95	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4(1)/a	
Unit cell dimensions	a = 23.7826(2)Å	a= 90°.
	b = 23.7826(2)Å	b = 90°.
	c = 31.3744(3)Å	g = 90°.
Volume	17745.7(3) $Å^3$	
Z	16	
Density (calculated)	1.340 Mg/m^3	
Absorption coefficient	3.357 mm^{-1}	
F(000)	7360	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	2.149 to 32.160°.	
Index ranges	-34<=h<=28,-33<=k<=34,-46<=l<=46	
Reflections collected	99138	
Independent reflections	14689[R(int) = 0.0567]	
Completeness to theta =32.160°	94.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.850 and 0.654	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14689/ 0/ 483	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0574	
R indices (all data)	R1 = 0.0642, wR2 = 0.0637	
Largest diff. peak and hole	0.658 and -0.607 e.$Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for SFC-A1.

Bond lengths----	
Au1-C28	1.983(3)
Au1-C1	2.015(2)
C1-N1	1.355(3)
C1-N2	1.355(3)
C2-C3	1.339(3)
C2-N2	1.391(3)
C2-H2	0.9500
C3-N1	1.380(3)

C3-H3	0.9500
C4-C9	1.395(4)
C4-C5	1.406(4)
C4-N1	1.451(3)
C5-C6	1.395(3)
C5-C10	1.508(4)
C6-C7	1.379(4)
C6-H6	0.9500
C7-C8	1.376(4)
C7-H7	0.9500
C8-C9	1.392(4)
C8-H8	0.9500
C9-C13	1.518(4)
C10-C12	1.528(4)
C10-C11	1.531(4)
C10-H10	1.0000
C11-H11A	0.9800
C11-H11B	0.9800
C11-H11C	0.9800
C12-H12A	0.9800
C12-H12B	0.9800
C12-H12C	0.9800
C13-C14	1.533(4)
C13-C15	1.533(4)
C13-H13	1.0000
C14-H14A	0.9800
C14-H14B	0.9800
C14-H14C	0.9800
C15-H15A	0.9800
C15-H15B	0.9800
C15-H15C	0.9800
C16-C21	1.393(4)
C16-C17	1.399(4)
C16-N2	1.441(3)
C17-C18	1.400(4)
C17-C22	1.510(4)
C18-C19	1.379(4)
C18-H18	0.9500

C19-C20	1.379(4)
C19-H19	0.9500
C20-C21	1.393(4)
C20-H20	0.9500
C21-C25	1.518(4)
C22-C24	1.529(4)
C22-C23	1.530(4)
C22-H22	1.0000
C23-H23A	0.9800
C23-H23B	0.9800
C23-H23C	0.9800
C24-H24A	0.9800
C24-H24B	0.9800
C24-H24C	0.9800
C25-C26	1.511(4)
C25-C27	1.516(5)
C25-H25	1.0000
C26-H26A	0.9800
C26-H26B	0.9800
C26-H26C	0.9800
C27-H27A	0.9800
C27-H27B	0.9800
C27-H27C	0.9800
C28-C29	1.206(3)
C29-C30	1.470(3)
C30-C31	1.542(3)
C30-H30A	0.9900
C30-H30B	0.9900
C31-C37	1.529(3)
C31-C39	1.531(3)
C31-C32	1.541(3)
C32-C33	1.501(3)
C32-H32A	0.9900
C32-H32B	0.9900
C33-C34	1.319(4)
C33-H33	0.9500
C34-C36	1.505(4)
C34-C35	1.506(4)

C35-H35A	0.9800
C35-H35B	0.9800
C35-H35C	0.9800
C36-H36A	0.9800
C36-H36B	0.9800
C36-H36C	0.9800
C37-O2	1.198(3)
C37-O1	1.337(3)
C38-O1	1.456(3)
C38-H38A	0.9800
C38-H38B	0.9800
C38-H38C	0.9800
C39-O4	1.199(3)
C39-O3	1.338(3)
C40-O3	1.457(3)
C40-H40A	0.9800
C40-H40B	0.9800
C40-H40C	0.9800
C1P-C2P	1.516(6)
C1P-H1P1	0.9800
C1P-H1P2	0.9800
C1P-H1P3	0.9800
C2P-C3P	1.444(5)
C2P-H2P1	0.9900
C2P-H2P2	0.9900
C3P-C4P	1.493(5)
C3P-H3P1	0.9900
C3P-H3P2	0.9900
C4P-C5P	1.526(6)
C4P-H4P1	0.9900
C4P-H4P2	0.9900
C5P-H5P1	0.9800
C5P-H5P2	0.9800
C5P-H5P3	0.9800

Angles----------

C28-Au1-C1	177.87(10)
N1-C1-N2	104.1(2)

N1-C1-Au1	128.63(17)
N2-C1-Au1	127.21(17)
C3-C2-N2	106.2(2)
C3-C2-H2	126.9
N2-C2-H2	126.9
C2-C3-N1	107.4(2)
C2-C3-H3	126.3
N1-C3-H3	126.3
C9-C4-C5	123.3(2)
C9-C4-N1	118.5(2)
C5-C4-N1	118.2(2)
C6-C5-C4	116.4(2)
C6-C5-C10	120.7(2)
C4-C5-C10	122.9(2)
C7-C6-C5	121.4(3)
C7-C6-H6	119.3
C5-C6-H6	119.3
C8-C7-C6	120.5(3)
C8-C7-H7	119.8
C6-C7-H7	119.8
C7-C8-C9	121.1(3)
C7-C8-H8	119.4
C9-C8-H8	119.4
C8-C9-C4	117.2(3)
C8-C9-C13	120.7(3)
C4-C9-C13	122.0(2)
C5-C10-C12	111.3(2)
C5-C10-C11	111.5(2)
C12-C10-C11	110.4(2)
C5-C10-H10	107.9
C12-C10-H10	107.9
C11-C10-H10	107.9
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5

C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C9-C13-C14	113.1(3)
C9-C13-C15	109.9(2)
C14-C13-C15	110.4(3)
C9-C13-H13	107.8
C14-C13-H13	107.8
C15-C13-H13	107.8
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C21-C16-C17	123.3(2)
C21-C16-N2	118.8(2)
C17-C16-N2	117.8(2)
C16-C17-C18	116.6(2)
C16-C17-C22	122.4(2)
C18-C17-C22	121.0(2)
C19-C18-C17	121.2(3)
C19-C18-H18	119.4
C17-C18-H18	119.4
C18-C19-C20	120.6(3)
C18-C19-H19	119.7
C20-C19-H19	119.7
C19-C20-C21	120.8(3)
C19-C20-H20	119.6

C21-C20-H20	119.6
C20-C21-C16	117.5(3)
C20-C21-C25	120.5(2)
C16-C21-C25	122.1(2)
C17-C22-C24	110.6(2)
C17-C22-C23	112.3(2)
C24-C22-C23	111.1(2)
C17-C22-H22	107.6
C24-C22-H22	107.6
C23-C22-H22	107.6
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C26-C25-C27	112.0(3)
C26-C25-C21	110.7(2)
C27-C25-C21	111.9(3)
C26-C25-H25	107.3
C27-C25-H25	107.3
C21-C25-H25	107.3
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5
C25-C27-H27C	109.5

H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
C29-C28-Au1	174.8(2)
C28-C29-C30	177.7(3)
C29-C30-C31	112.9(2)
C29-C30-H30A	109.0
C31-C30-H30A	109.0
C29-C30-H30B	109.0
C31-C30-H30B	109.0
H30A-C30-H30B	107.8
C37-C31-C39	107.73(19)
C37-C31-C32	110.6(2)
C39-C31-C32	109.99(19)
C37-C31-C30	108.19(19)
C39-C31-C30	108.99(19)
C32-C31-C30	111.25(19)
C33-C32-C31	113.0(2)
C33-C32-H32A	109.0
C31-C32-H32A	109.0
C33-C32-H32B	109.0
C31-C32-H32B	109.0
H32A-C32-H32B	107.8
C34-C33-C32	128.5(3)
C34-C33-H33	115.7
C32-C33-H33	115.7
C33-C34-C36	121.6(3)
C33-C34-C35	124.4(3)
C36-C34-C35	114.1(3)
C34-C35-H35A	109.5
C34-C35-H35B	109.5
H35A-C35-H35B	109.5
C34-C35-H35C	109.5
H35A-C35-H35C	109.5
H35B-C35-H35C	109.5
C34-C36-H36A	109.5
C34-C36-H36B	109.5
H36A-C36-H36B	109.5
C34-C36-H36C	109.5

H36A-C36-H36C	109.5
H36B-C36-H36C	109.5
O2-C37-O1	123.6(2)
O2-C37-C31	125.4(2)
O1-C37-C31	111.0(2)
O1-C38-H38A	109.5
O1-C38-H38B	109.5
H38A-C38-H38B	109.5
O1-C38-H38C	109.5
H38A-C38-H38C	109.5
H38B-C38-H38C	109.5
O4-C39-O3	124.8(2)
O4-C39-C31	125.6(2)
O3-C39-C31	109.6(2)
O3-C40-H40A	109.5
O3-C40-H40B	109.5
H40A-C40-H40B	109.5
O3-C40-H40C	109.5
H40A-C40-H40C	109.5
H40B-C40-H40C	109.5
C2P-C1P-H1P1	109.5
C2P-C1P-H1P2	109.5
H1P1-C1P-H1P2	109.5
C2P-C1P-H1P3	109.5
H1P1-C1P-H1P3	109.5
H1P2-C1P-H1P3	109.5
C3P-C2P-C1P	110.5(3)
C3P-C2P-H2P1	109.5
C1P-C2P-H2P1	109.5
C3P-C2P-H2P2	109.5
C1P-C2P-H2P2	109.5
H2P1-C2P-H2P2	108.1
C2P-C3P-C4P	112.6(3)
C2P-C3P-H3P1	109.1
C4P-C3P-H3P1	109.1
C2P-C3P-H3P2	109.1
C4P-C3P-H3P2	109.1
H3P1-C3P-H3P2	107.8

C3P-C4P-C5P	111.5(4)
C3P-C4P-H4P1	109.3
C5P-C4P-H4P1	109.3
C3P-C4P-H4P2	109.3
C5P-C4P-H4P2	109.3
H4P1-C4P-H4P2	108.0
C4P-C5P-H5P1	109.5
C4P-C5P-H5P2	109.5
H5P1-C5P-H5P2	109.5
C4P-C5P-H5P3	109.5
H5P1-C5P-H5P3	109.5
H5P2-C5P-H5P3	109.5
C1-N1-C3	111.1(2)
C1-N1-C4	123.2(2)
C3-N1-C4	125.7(2)
C1-N2-C2	111.2(2)
C1-N2-C16	123.2(2)
C2-N2-C16	125.6(2)
C37-O1-C38	114.6(2)
C39-O3-C40	115.7(2)

Table 3. Torsion angles [°] for SFC-A1.

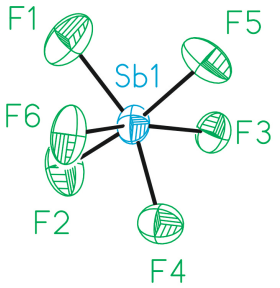
N2-C2-C3-N1	-0.2(3)
C9-C4-C5-C6	-2.3(4)
N1-C4-C5-C6	176.8(2)
C9-C4-C5-C10	176.9(2)
N1-C4-C5-C10	-4.1(4)
C4-C5-C6-C7	1.4(4)
C10-C5-C6-C7	-177.7(2)
C5-C6-C7-C8	0.5(4)
C6-C7-C8-C9	-1.8(4)
C7-C8-C9-C4	1.0(4)
C7-C8-C9-C13	-175.7(3)
C5-C4-C9-C8	1.1(4)
N1-C4-C9-C8	-178.0(2)
C5-C4-C9-C13	177.7(2)
N1-C4-C9-C13	-1.3(4)

C6-C5-C10-C12	62.0(3)
C4-C5-C10-C12	-117.1(3)
C6-C5-C10-C11	-61.7(3)
C4-C5-C10-C11	119.2(3)
C8-C9-C13-C14	-42.7(4)
C4-C9-C13-C14	140.8(3)
C8-C9-C13-C15	81.1(3)
C4-C9-C13-C15	-95.3(3)
C21-C16-C17-C18	-2.0(4)
N2-C16-C17-C18	177.4(2)
C21-C16-C17-C22	177.1(2)
N2-C16-C17-C22	-3.5(4)
C16-C17-C18-C19	0.3(4)
C22-C17-C18-C19	-178.8(3)
C17-C18-C19-C20	1.2(4)
C18-C19-C20-C21	-1.0(4)
C19-C20-C21-C16	-0.6(4)
C19-C20-C21-C25	177.9(2)
C17-C16-C21-C20	2.2(4)
N2-C16-C21-C20	-177.2(2)
C17-C16-C21-C25	-176.3(2)
N2-C16-C21-C25	4.3(4)
C16-C17-C22-C24	-121.3(3)
C18-C17-C22-C24	57.7(3)
C16-C17-C22-C23	114.0(3)
C18-C17-C22-C23	-67.0(3)
C20-C21-C25-C26	-64.5(3)
C16-C21-C25-C26	114.0(3)
C20-C21-C25-C27	61.2(4)
C16-C21-C25-C27	-120.4(4)
C29-C30-C31-C37	174.57(19)
C29-C30-C31-C39	57.7(3)
C29-C30-C31-C32	-63.8(3)
C37-C31-C32-C33	54.9(3)
C39-C31-C32-C33	173.7(2)
C30-C31-C32-C33	-65.4(3)
C31-C32-C33-C34	116.0(3)
C32-C33-C34-C36	177.3(3)

C32-C33-C34-C35	-1.6(5)
C39-C31-C37-O2	121.4(3)
C32-C31-C37-O2	-118.4(3)
C30-C31-C37-O2	3.7(3)
C39-C31-C37-O1	-59.7(3)
C32-C31-C37-O1	60.5(3)
C30-C31-C37-O1	-177.39(19)
C37-C31-C39-O4	123.1(3)
C32-C31-C39-O4	2.5(3)
C30-C31-C39-O4	-119.7(3)
C37-C31-C39-O3	-57.4(3)
C32-C31-C39-O3	-177.99(19)
C30-C31-C39-O3	59.8(2)
C1P-C2P-C3P-C4P	179.7(3)
C2P-C3P-C4P-C5P	-175.3(3)
N2-C1-N1-C3	0.7(3)
Au1-C1-N1-C3	179.43(18)
N2-C1-N1-C4	179.4(2)
Au1-C1-N1-C4	-1.8(4)
C2-C3-N1-C1	-0.3(3)
C2-C3-N1-C4	-179.0(2)
C9-C4-N1-C1	101.5(3)
C5-C4-N1-C1	-77.6(3)
C9-C4-N1-C3	-79.9(3)
C5-C4-N1-C3	101.0(3)
N1-C1-N2-C2	-0.8(3)
Au1-C1-N2-C2	-179.57(18)
N1-C1-N2-C16	178.4(2)
Au1-C1-N2-C16	-0.4(3)
C3-C2-N2-C1	0.6(3)
C3-C2-N2-C16	-178.6(2)
C21-C16-N2-C1	95.5(3)
C17-C16-N2-C1	-83.9(3)
C21-C16-N2-C2	-85.4(3)
C17-C16-N2-C2	95.1(3)
O2-C37-O1-C38	0.2(4)
C31-C37-O1-C38	-178.7(2)
O4-C39-O3-C40	4.6(4)

C31-C39-O3-C40 -174.9(2)

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (14a) CCDC 1572066.



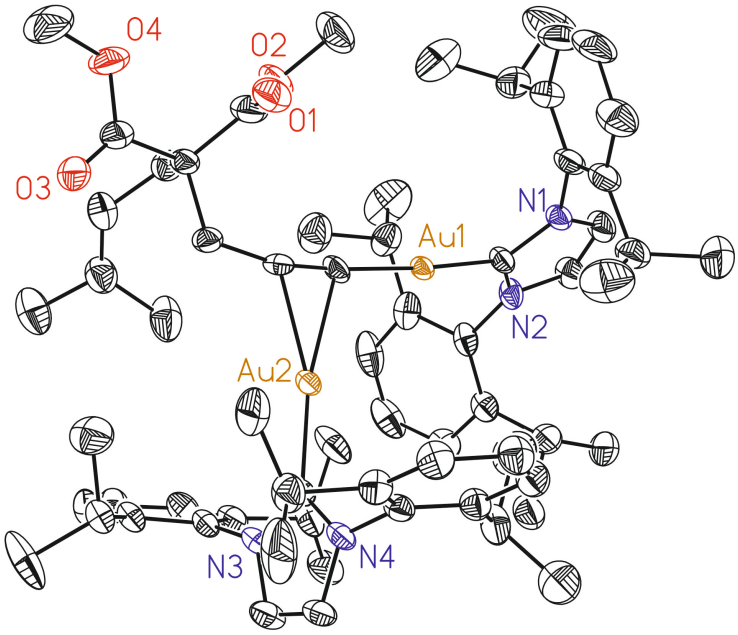


Table 1. Crystal data and structure refinement for SFC-A-13_twin1_hklf5.

Identification code	SFC-A-13_twin1_hklf5	
Empirical formula	C70 H92 Au2 Cl9 F6 N4 O4 Sb	
Formula weight	2002.20	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.55234(18)Å	⟨= 84.3516(9)°.
	b = 18.1401(3)Å	® = 77.7749(10)°.
	c = 18.30982(17)Å	© = 88.2220(12)°.
Volume	4054.60(9) Å^3	

Z	2
Density (calculated)	1.640 Mg/m^3
Absorption coefficient	4.296 mm^{-1}
F(000)	1976
Crystal size	0.10 x 0.04 x 0.01 mm^3
Theta range for data collection	2.257 to 34.963°.
Index ranges	-19<=h<=19,-28<=k<=29,-28<=l<=29
Reflections collected	66445
Independent reflections	66445[R(int) =?]
Completeness to theta =34.963°	94.3%
Absorption correction	Empirical
Max. and min. transmission	0.919 and 0.707
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	66445/ 387/ 976
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0995, wR2 = 0.2561
R indices (all data)	R1 = 0.1486, wR2 = 0.2894
Largest diff. peak and hole	6.594 and -4.757 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for SFC-A-13_twin1_hklf5.

Bond lengths----

Au1-C55	2.002(8)
Au1-C1	2.011(8)
Au2-C28	1.990(8)
Au2-C56	2.202(7)
Au2-C55	2.251(7)
N1-C1	1.360(10)
N1-C2	1.406(11)
N1-C4	1.449(11)
N2-C1	1.353(11)
N2-C3	1.382(11)
N2-C16	1.431(11)
N3-C28	1.367(9)
N3-C29	1.405(11)
N3-C31	1.440(11)
N4-C28	1.347(10)
N4-C30	1.392(10)
N4-C43	1.452(10)

O1-C59	1.191(12)
O2-C59	1.324(12)
O2-C60	1.416(13)
O3-C61	1.194(11)
O4-C61	1.344(11)
O4-C62	1.463(14)
C2-C3	1.339(14)
C2-H2	0.9300
C3-H3	0.9300
C4-C5	1.376(14)
C4-C9	1.396(13)
C5-C6	1.398(14)
C5-C10	1.506(14)
C6-C7	1.407(18)
C6-H6	0.9300
C7-C8	1.35(2)
C7-H7	0.9300
C8-C9	1.404(15)
C8-H8	0.9300
C9-C13	1.526(16)
C10-C11	1.530(17)
C10-C12	1.531(16)
C10-H10	0.9800
C11-H11A	0.9600
C11-H11B	0.9600
C11-H11C	0.9600
C12-H12A	0.9600
C12-H12B	0.9600
C12-H12C	0.9600
C13-C14	1.521(19)
C13-C15	1.530(17)
C13-H13	0.9800
C14-H14A	0.9600
C14-H14B	0.9600
C14-H14C	0.9600
C15-H15A	0.9600
C15-H15B	0.9600
C15-H15C	0.9600

C16-C17	1.396(13)
C16-C21	1.417(12)
C17-C18	1.399(13)
C17-C22	1.513(14)
C18-C19	1.377(16)
C18-H18	0.9300
C19-C20	1.369(18)
C19-H19	0.9300
C20-C21	1.424(14)
C20-H20	0.9300
C21-C25	1.494(15)
C22-C23	1.508(14)
C22-C24	1.575(15)
C22-H22	0.9800
C23-H23A	0.9600
C23-H23B	0.9600
C23-H23C	0.9600
C24-H24A	0.9600
C24-H24B	0.9600
C24-H24C	0.9600
C25-C26	1.521(15)
C25-C27	1.554(16)
C25-H25	0.9800
C26-H26A	0.9600
C26-H26B	0.9600
C26-H26C	0.9600
C27-H27A	0.9600
C27-H27B	0.9600
C27-H27C	0.9600
C29-C30	1.339(13)
C29-H29	0.9300
C30-H30	0.9300
C31-C32	1.395(12)
C31-C36	1.408(12)
C32-C33	1.423(13)
C32-C37	1.497(13)
C33-C34	1.354(14)
C33-H33	0.9300

C34-C35	1.372(14)
C34-H34	0.9300
C35-C36	1.410(12)
C35-H35	0.9300
C36-C40	1.521(13)
C37-C38	1.511(14)
C37-C39	1.536(14)
C37-H37	0.9800
C38-H38A	0.9600
C38-H38B	0.9600
C38-H38C	0.9600
C39-H39A	0.9600
C39-H39B	0.9600
C39-H39C	0.9600
C40-C41	1.511(14)
C40-C42	1.528(13)
C40-H40	0.9800
C41-H41A	0.9600
C41-H41B	0.9600
C41-H41C	0.9600
C42-H42A	0.9600
C42-H42B	0.9600
C42-H42C	0.9600
C43-C44	1.391(12)
C43-C48	1.392(12)
C44-C45	1.389(13)
C44-C49	1.518(13)
C45-C46	1.379(13)
C45-H45	0.9300
C46-C47	1.402(14)
C46-H46	0.9300
C47-C48	1.387(13)
C47-H47	0.9300
C48-C52	1.527(13)
C49-C50	1.526(16)
C49-C51	1.528(16)
C49-H49	0.9800
C50-H50A	0.9600

C50-H50B	0.9600
C50-H50C	0.9600
C51-H51A	0.9600
C51-H51B	0.9600
C51-H51C	0.9600
C52-C53	1.499(16)
C52-C54	1.555(15)
C52-H52	0.9800
C53-H53A	0.9600
C53-H53B	0.9600
C53-H53C	0.9600
C54-H54A	0.9600
C54-H54B	0.9600
C54-H54C	0.9600
C55-C56	1.226(11)
C56-C57	1.468(12)
C57-C58	1.574(12)
C57-H57A	0.9700
C57-H57B	0.9700
C58-C63	1.519(13)
C58-C59	1.527(13)
C58-C61	1.531(13)
C60-H60A	0.9600
C60-H60B	0.9600
C60-H60C	0.9600
C62-H62A	0.9600
C62-H62B	0.9600
C62-H62C	0.9600
C63-C64	1.517(14)
C63-H63A	0.9700
C63-H63B	0.9700
C64-C65	1.323(15)
C64-H64	0.9300
C65-C67	1.478(15)
C65-C66	1.530(16)
C66-H66A	0.9600
C66-H66B	0.9600
C66-H66C	0.9600

C67-H67A	0.9600
C67-H67B	0.9600
C67-H67C	0.9600
Sb1-F4	1.813(11)
Sb1-F5	1.834(12)
Sb1-F1	1.854(11)
Sb1-F2	1.858(10)
Sb1-F3	1.918(11)
Sb1-F6	1.946(11)
Sb1'-F4'	1.834(11)
Sb1'-F2'	1.842(10)
Sb1'-F1'	1.842(11)
Sb1'-F5'	1.845(11)
Sb1'-F3'	1.924(11)
Sb1'-F6'	1.949(11)
C1S-Cl1S	1.705(13)
C1S-Cl2S	1.717(13)
C1S-Cl3S	1.778(15)
C1S-H1S	0.9800
C1T-Cl3T	1.727(15)
C1T-Cl1T	1.755(14)
C1T-Cl2T	1.775(17)
C1T-H1T	0.9800
C1T'-Cl3'	1.726(16)
C1T'-Cl1'	1.754(16)
C1T'-Cl2'	1.775(18)
C1T'-H1T'	0.9800
C1U-Cl1U	1.723(15)
C1U-Cl2U	1.779(13)
C1U-Cl3U	1.788(14)
C1U-H1U	0.9800

Angles----------

C55-Au1-C1	175.7(3)
C28-Au2-C56	160.7(3)
C28-Au2-C55	167.0(3)
C56-Au2-C55	31.9(3)
C1-N1-C2	110.2(7)

C1-N1-C4	125.4(7)
C2-N1-C4	123.7(7)
C1-N2-C3	111.0(7)
C1-N2-C16	128.4(7)
C3-N2-C16	120.4(7)
C28-N3-C29	109.9(7)
C28-N3-C31	127.5(7)
C29-N3-C31	122.6(7)
C28-N4-C30	111.3(7)
C28-N4-C43	125.1(6)
C30-N4-C43	123.6(7)
C59-O2-C60	115.7(10)
C61-O4-C62	114.1(9)
N2-C1-N1	104.9(7)
N2-C1-Au1	129.4(6)
N1-C1-Au1	125.7(6)
C3-C2-N1	106.4(8)
C3-C2-H2	126.8
N1-C2-H2	126.8
C2-C3-N2	107.5(8)
C2-C3-H3	126.3
N2-C3-H3	126.3
C5-C4-C9	125.4(9)
C5-C4-N1	118.8(8)
C9-C4-N1	115.7(9)
C4-C5-C6	116.2(10)
C4-C5-C10	123.1(8)
C6-C5-C10	120.6(10)
C5-C6-C7	120.9(12)
C5-C6-H6	119.5
C7-C6-H6	119.5
C8-C7-C6	119.5(10)
C8-C7-H7	120.3
C6-C7-H7	120.3
C7-C8-C9	123.0(11)
C7-C8-H8	118.5
C9-C8-H8	118.5
C4-C9-C8	114.9(11)

C4-C9-C13	123.0(9)
C8-C9-C13	122.1(10)
C5-C10-C11	111.7(10)
C5-C10-C12	111.5(9)
C11-C10-C12	110.8(12)
C5-C10-H10	107.5
C11-C10-H10	107.5
C12-C10-H10	107.5
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5
H11B-C11-H11C	109.5
C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C14-C13-C9	111.0(11)
C14-C13-C15	107.3(12)
C9-C13-C15	112.2(11)
C14-C13-H13	108.8
C9-C13-H13	108.8
C15-C13-H13	108.8
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5

C17-C16-C21	123.1(8)
C17-C16-N2	119.7(8)
C21-C16-N2	116.9(8)
C16-C17-C18	117.8(9)
C16-C17-C22	121.9(8)
C18-C17-C22	120.3(9)
C19-C18-C17	120.9(10)
C19-C18-H18	119.6
C17-C18-H18	119.6
C20-C19-C18	121.0(9)
C20-C19-H19	119.5
C18-C19-H19	119.5
C19-C20-C21	121.4(10)
C19-C20-H20	119.3
C21-C20-H20	119.3
C16-C21-C20	115.8(10)
C16-C21-C25	124.4(9)
C20-C21-C25	119.8(9)
C23-C22-C17	112.7(9)
C23-C22-C24	107.6(8)
C17-C22-C24	111.3(8)
C23-C22-H22	108.4
C17-C22-H22	108.4
C24-C22-H22	108.4
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C21-C25-C26	113.4(10)
C21-C25-C27	111.4(9)

C26-C25-C27	109.8(10)
C21-C25-H25	107.3
C26-C25-H25	107.3
C27-C25-H25	107.3
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5
C25-C27-H27C	109.5
H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
N4-C28-N3	105.0(6)
N4-C28-Au2	128.5(6)
N3-C28-Au2	126.5(6)
C30-C29-N3	107.0(8)
C30-C29-H29	126.5
N3-C29-H29	126.5
C29-C30-N4	106.8(8)
C29-C30-H30	126.6
N4-C30-H30	126.6
C32-C31-C36	123.7(8)
C32-C31-N3	118.9(8)
C36-C31-N3	117.3(7)
C31-C32-C33	117.2(9)
C31-C32-C37	123.4(8)
C33-C32-C37	119.4(8)
C34-C33-C32	120.0(9)
C34-C33-H33	120.0
C32-C33-H33	120.0
C33-C34-C35	121.7(9)
C33-C34-H34	119.1
C35-C34-H34	119.1
C34-C35-C36	121.8(9)

C34-C35-H35	119.1
C36-C35-H35	119.1
C31-C36-C35	115.4(8)
C31-C36-C40	122.9(8)
C35-C36-C40	121.6(8)
C32-C37-C38	109.7(9)
C32-C37-C39	112.8(8)
C38-C37-C39	110.1(9)
C32-C37-H37	108.0
C38-C37-H37	108.0
C39-C37-H37	108.0
C37-C38-H38A	109.5
C37-C38-H38B	109.5
H38A-C38-H38B	109.5
C37-C38-H38C	109.5
H38A-C38-H38C	109.5
H38B-C38-H38C	109.5
C37-C39-H39A	109.5
C37-C39-H39B	109.5
H39A-C39-H39B	109.5
C37-C39-H39C	109.5
H39A-C39-H39C	109.5
H39B-C39-H39C	109.5
C41-C40-C36	110.1(8)
C41-C40-C42	111.5(10)
C36-C40-C42	111.4(8)
C41-C40-H40	107.9
C36-C40-H40	107.9
C42-C40-H40	107.9
C40-C41-H41A	109.5
C40-C41-H41B	109.5
H41A-C41-H41B	109.5
C40-C41-H41C	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
C40-C42-H42A	109.5
C40-C42-H42B	109.5
H42A-C42-H42B	109.5

C40-C42-H42C	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
C44-C43-C48	123.7(8)
C44-C43-N4	118.5(7)
C48-C43-N4	117.8(8)
C45-C44-C43	117.2(8)
C45-C44-C49	120.3(8)
C43-C44-C49	122.4(8)
C46-C45-C44	121.6(9)
C46-C45-H45	119.2
C44-C45-H45	119.2
C45-C46-C47	119.1(9)
C45-C46-H46	120.5
C47-C46-H46	120.5
C48-C47-C46	121.6(9)
C48-C47-H47	119.2
C46-C47-H47	119.2
C47-C48-C43	116.7(8)
C47-C48-C52	120.3(8)
C43-C48-C52	122.9(8)
C44-C49-C50	112.1(9)
C44-C49-C51	109.2(8)
C50-C49-C51	111.2(9)
C44-C49-H49	108.1
C50-C49-H49	108.1
C51-C49-H49	108.1
C49-C50-H50A	109.5
C49-C50-H50B	109.5
H50A-C50-H50B	109.5
C49-C50-H50C	109.5
H50A-C50-H50C	109.5
H50B-C50-H50C	109.5
C49-C51-H51A	109.5
C49-C51-H51B	109.5
H51A-C51-H51B	109.5
C49-C51-H51C	109.5
H51A-C51-H51C	109.5

H51B-C51-H51C	109.5
C53-C52-C48	112.3(9)
C53-C52-C54	109.1(11)
C48-C52-C54	110.6(9)
C53-C52-H52	108.2
C48-C52-H52	108.2
C54-C52-H52	108.2
C52-C53-H53A	109.5
C52-C53-H53B	109.5
H53A-C53-H53B	109.5
C52-C53-H53C	109.5
H53A-C53-H53C	109.5
H53B-C53-H53C	109.5
C52-C54-H54A	109.5
C52-C54-H54B	109.5
H54A-C54-H54B	109.5
C52-C54-H54C	109.5
H54A-C54-H54C	109.5
H54B-C54-H54C	109.5
C56-C55-Au1	173.0(7)
C56-C55-Au2	71.8(5)
Au1-C55-Au2	113.7(4)
C55-C56-C57	165.7(8)
C55-C56-Au2	76.2(5)
C57-C56-Au2	117.9(5)
C56-C57-C58	111.5(7)
C56-C57-H57A	109.3
C58-C57-H57A	109.3
C56-C57-H57B	109.3
C58-C57-H57B	109.3
H57A-C57-H57B	108.0
C63-C58-C59	113.2(7)
C63-C58-C61	111.2(8)
C59-C58-C61	107.2(7)
C63-C58-C57	112.5(7)
C59-C58-C57	106.0(8)
C61-C58-C57	106.1(7)
O1-C59-O2	125.0(10)

O1-C59-C58	123.3(9)
O2-C59-C58	111.7(9)
O2-C60-H60A	109.5
O2-C60-H60B	109.5
H60A-C60-H60B	109.5
O2-C60-H60C	109.5
H60A-C60-H60C	109.5
H60B-C60-H60C	109.5
O3-C61-O4	124.9(9)
O3-C61-C58	126.3(8)
O4-C61-C58	108.7(8)
O4-C62-H62A	109.5
O4-C62-H62B	109.5
H62A-C62-H62B	109.5
O4-C62-H62C	109.5
H62A-C62-H62C	109.5
H62B-C62-H62C	109.5
C64-C63-C58	113.8(8)
C64-C63-H63A	108.8
C58-C63-H63A	108.8
C64-C63-H63B	108.8
C58-C63-H63B	108.8
H63A-C63-H63B	107.7
C65-C64-C63	128.7(10)
C65-C64-H64	115.7
C63-C64-H64	115.7
C64-C65-C67	121.1(11)
C64-C65-C66	125.4(10)
C67-C65-C66	113.4(10)
C65-C66-H66A	109.5
C65-C66-H66B	109.5
H66A-C66-H66B	109.5
C65-C66-H66C	109.5
H66A-C66-H66C	109.5
H66B-C66-H66C	109.5
C65-C67-H67A	109.5
C65-C67-H67B	109.5
H67A-C67-H67B	109.5

C65-C67-H67C	109.5
H67A-C67-H67C	109.5
H67B-C67-H67C	109.5
F4-Sb1-F5	102.7(6)
F4-Sb1-F1	158.3(6)
F5-Sb1-F1	93.5(6)
F4-Sb1-F2	89.8(6)
F5-Sb1-F2	165.0(6)
F1-Sb1-F2	76.6(6)
F4-Sb1-F3	89.2(6)
F5-Sb1-F3	83.0(6)
F1-Sb1-F3	107.1(6)
F2-Sb1-F3	89.1(5)
F4-Sb1-F6	77.2(6)
F5-Sb1-F6	91.4(6)
F1-Sb1-F6	88.2(5)
F2-Sb1-F6	99.4(5)
F3-Sb1-F6	163.9(6)
F4'-Sb1'-F2'	89.4(6)
F4'-Sb1'-F1'	159.6(6)
F2'-Sb1'-F1'	80.6(6)
F4'-Sb1'-F5'	100.5(6)
F2'-Sb1'-F5'	166.1(6)
F1'-Sb1'-F5'	92.7(6)
F4'-Sb1'-F3'	87.3(6)
F2'-Sb1'-F3'	89.7(5)
F1'-Sb1'-F3'	110.3(6)
F5'-Sb1'-F3'	81.1(5)
F4'-Sb1'-F6'	75.4(6)
F2'-Sb1'-F6'	100.6(6)
F1'-Sb1'-F6'	88.9(6)
F5'-Sb1'-F6'	91.4(6)
F3'-Sb1'-F6'	159.6(6)
Cl1S-C1S-Cl2S	115.7(9)
Cl1S-C1S-Cl3S	109.7(7)
Cl2S-C1S-Cl3S	107.3(7)
Cl1S-C1S-H1S	107.9
Cl2S-C1S-H1S	107.9

Cl3S-C1S-H1S	107.9
Cl3T-C1T-Cl1T	111.9(9)
Cl3T-C1T-Cl2T	109.4(8)
Cl1T-C1T-Cl2T	112.5(8)
Cl3T-C1T-H1T	107.6
Cl1T-C1T-H1T	107.6
Cl2T-C1T-H1T	107.6
Cl3'-C1T'-Cl1'	112.3(13)
Cl3'-C1T'-Cl2'	109.5(12)
Cl1'-C1T'-Cl2'	112.8(12)
Cl3'-C1T'-H1T'	107.3
Cl1'-C1T'-H1T'	107.3
Cl2'-C1T'-H1T'	107.3
Cl1U-C1U-Cl2U	111.6(7)
Cl1U-C1U-Cl3U	110.2(7)
Cl2U-C1U-Cl3U	108.6(8)
Cl1U-C1U-H1U	108.8
Cl2U-C1U-H1U	108.8
Cl3U-C1U-H1U	108.8

Table 3. Torsion angles [°] for SFC-A-13_twin1_hklf5.

C3-N2-C1-N1	-1.1(10)
C16-N2-C1-N1	-175.0(8)
C3-N2-C1-Au1	179.6(7)
C16-N2-C1-Au1	5.7(14)
C2-N1-C1-N2	0.3(10)
C4-N1-C1-N2	171.6(8)
C2-N1-C1-Au1	179.7(7)
C4-N1-C1-Au1	-9.0(12)
C1-N1-C2-C3	0.6(11)
C4-N1-C2-C3	-170.9(9)
N1-C2-C3-N2	-1.2(11)
C1-N2-C3-C2	1.4(11)
C16-N2-C3-C2	175.9(8)
C1-N1-C4-C5	89.8(11)
C2-N1-C4-C5	-100.1(11)
C1-N1-C4-C9	-93.1(11)

C2-N1-C4-C9	77.0(12)
C9-C4-C5-C6	0.5(15)
N1-C4-C5-C6	177.3(9)
C9-C4-C5-C10	-176.4(10)
N1-C4-C5-C10	0.4(14)
C4-C5-C6-C7	-0.4(16)
C10-C5-C6-C7	176.6(11)
C5-C6-C7-C8	0.2(19)
C6-C7-C8-C9	0(2)
C5-C4-C9-C8	-0.4(16)
N1-C4-C9-C8	-177.3(9)
C5-C4-C9-C13	178.0(10)
N1-C4-C9-C13	1.1(14)
C7-C8-C9-C4	0.1(18)
C7-C8-C9-C13	-178.3(12)
C4-C5-C10-C11	-129.3(11)
C6-C5-C10-C11	54.0(14)
C4-C5-C10-C12	106.0(13)
C6-C5-C10-C12	-70.7(15)
C4-C9-C13-C14	114.0(13)
C8-C9-C13-C14	-67.7(15)
C4-C9-C13-C15	-126.0(13)
C8-C9-C13-C15	52.3(17)
C1-N2-C16-C17	-115.9(10)
C3-N2-C16-C17	70.7(11)
C1-N2-C16-C21	70.7(11)
C3-N2-C16-C21	-102.7(10)
C21-C16-C17-C18	1.4(13)
N2-C16-C17-C18	-171.6(8)
C21-C16-C17-C22	-175.7(8)
N2-C16-C17-C22	11.4(12)
C16-C17-C18-C19	-1.1(14)
C22-C17-C18-C19	176.0(9)
C17-C18-C19-C20	0.3(16)
C18-C19-C20-C21	0.3(16)
C17-C16-C21-C20	-0.9(13)
N2-C16-C21-C20	172.3(8)
C17-C16-C21-C25	-178.9(8)

N2-C16-C21-C25	-5.7(12)
C19-C20-C21-C16	0.0(14)
C19-C20-C21-C25	178.1(9)
C16-C17-C22-C23	-107.3(10)
C18-C17-C22-C23	75.8(12)
C16-C17-C22-C24	131.7(9)
C18-C17-C22-C24	-45.2(12)
C16-C21-C25-C26	115.6(12)
C20-C21-C25-C26	-62.4(14)
C16-C21-C25-C27	-120.0(10)
C20-C21-C25-C27	62.1(12)
C30-N4-C28-N3	0.1(10)
C43-N4-C28-N3	-178.5(7)
C30-N4-C28-Au2	179.2(7)
C43-N4-C28-Au2	0.5(12)
C29-N3-C28-N4	-1.3(9)
C31-N3-C28-N4	-179.4(8)
C29-N3-C28-Au2	179.6(6)
C31-N3-C28-Au2	1.5(12)
C28-N3-C29-C30	2.0(11)
C31-N3-C29-C30	-179.8(8)
N3-C29-C30-N4	-1.8(11)
C28-N4-C30-C29	1.1(11)
C43-N4-C30-C29	179.8(8)
C28-N3-C31-C32	83.0(11)
C29-N3-C31-C32	-94.9(10)
C28-N3-C31-C36	-100.4(10)
C29-N3-C31-C36	81.7(11)
C36-C31-C32-C33	-1.9(13)
N3-C31-C32-C33	174.4(7)
C36-C31-C32-C37	174.6(8)
N3-C31-C32-C37	-9.0(12)
C31-C32-C33-C34	-1.3(13)
C37-C32-C33-C34	-178.0(9)
C32-C33-C34-C35	4.3(15)
C33-C34-C35-C36	-4.2(16)
C32-C31-C36-C35	2.1(13)
N3-C31-C36-C35	-174.3(8)

C32-C31-C36-C40	-174.8(8)
N3-C31-C36-C40	8.8(12)
C34-C35-C36-C31	1.0(14)
C34-C35-C36-C40	177.8(9)
C31-C32-C37-C38	-103.1(10)
C33-C32-C37-C38	73.4(11)
C31-C32-C37-C39	133.8(10)
C33-C32-C37-C39	-49.7(13)
C31-C36-C40-C41	94.0(11)
C35-C36-C40-C41	-82.6(11)
C31-C36-C40-C42	-141.7(10)
C35-C36-C40-C42	41.6(13)
C28-N4-C43-C44	-90.2(10)
C30-N4-C43-C44	91.3(10)
C28-N4-C43-C48	91.9(10)
C30-N4-C43-C48	-86.6(11)
C48-C43-C44-C45	-0.5(13)
N4-C43-C44-C45	-178.3(8)
C48-C43-C44-C49	-178.7(9)
N4-C43-C44-C49	3.4(13)
C43-C44-C45-C46	-0.3(14)
C49-C44-C45-C46	178.0(9)
C44-C45-C46-C47	0.7(15)
C45-C46-C47-C48	-0.4(15)
C46-C47-C48-C43	-0.3(14)
C46-C47-C48-C52	179.2(9)
C44-C43-C48-C47	0.8(13)
N4-C43-C48-C47	178.6(8)
C44-C43-C48-C52	-178.7(9)
N4-C43-C48-C52	-0.9(12)
C45-C44-C49-C50	53.8(13)
C43-C44-C49-C50	-127.9(10)
C45-C44-C49-C51	-69.9(12)
C43-C44-C49-C51	108.4(10)
C47-C48-C52-C53	64.7(13)
C43-C48-C52-C53	-115.8(12)
C47-C48-C52-C54	-57.4(13)
C43-C48-C52-C54	122.0(12)

Au2-C55-C56-C57	-170(4)
C55-C56-C57-C58	5(4)
Au2-C56-C57-C58	-164.6(6)
C56-C57-C58-C63	68.2(10)
C56-C57-C58-C59	-56.1(9)
C56-C57-C58-C61	-169.9(8)
C60-O2-C59-O1	0.5(16)
C60-O2-C59-C58	180.0(9)
C63-C58-C59-O1	177.2(9)
C61-C58-C59-O1	54.1(13)
C57-C58-C59-O1	-59.0(12)
C63-C58-C59-O2	-2.3(12)
C61-C58-C59-O2	-125.4(9)
C57-C58-C59-O2	121.6(9)
C62-O4-C61-O3	9.6(17)
C62-O4-C61-C58	-173.7(11)
C63-C58-C61-O3	101.4(12)
C59-C58-C61-O3	-134.4(11)
C57-C58-C61-O3	-21.4(14)
C63-C58-C61-O4	-75.3(10)
C59-C58-C61-O4	48.9(11)
C57-C58-C61-O4	161.9(8)
C59-C58-C63-C64	-175.7(8)
C61-C58-C63-C64	-54.9(10)
C57-C58-C63-C64	64.1(10)
C58-C63-C64-C65	-104.9(13)
C63-C64-C65-C67	179.1(11)
C63-C64-C65-C66	2.2(19)

{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (14b) CCDC 1572071.

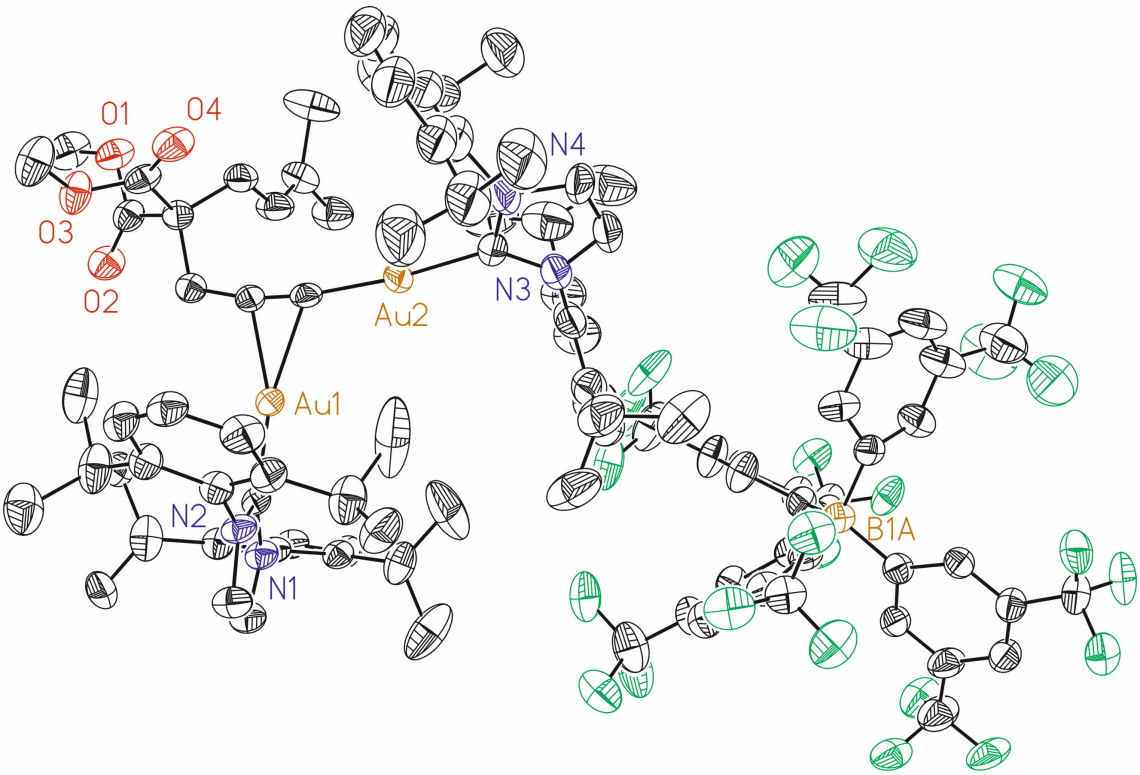


Table 1. Crystal data and structure refinement for SCF-A-14_twin1_hklf5.

Identification code	SCF-A-14_twin1_hklf5	
Empirical formula	C49.50 H50.50 Au B0.50 F12 N2 O2	
Formula weight	1135.79	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 15.9112(3)Å	a= 87.5507(12)°.
	b = 16.9278(3)Å	b = 77.7533(13)°.
	c = 19.2119(3)Å	g = 88.0670(13)°.
Volume	5050.57(14) $Å^3$	
Z	4	
Density (calculated)	1.494 Mg/m^3	
Absorption coefficient	2.996 mm^{-1}	
F(000)	2268	
Crystal size	?0.10 x 0.08 x 0.05 mm^3	
Theta range for data collection	2.220 to 37.502°.	
Index ranges	-27<=h<=27,-28<=k<=28,-32<=l<=32	
Reflections collected	192681	
Independent reflections	192681[R(int) =?]	

Completeness to theta =37.502°	97.2%
Absorption correction	Empirical
Max. and min. transmission	0.865 and 0.665
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	192681/ 2687/ 1741
Goodness-of-fit on F^2	0.866
Final R indices [I>2sigma(I)]	R1 = 0.0977, wR2 = 0.2487
R indices (all data)	R1 = 0.2771, wR2 = 0.3169
Largest diff. peak and hole	5.566 and -3.294 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for SCF-A-14_twin1_hklf5.

Bond lengths----

Au1-C1	1.986(8)
Au1-C55	2.208(8)
Au1-C56	2.226(9)
Au2-C55	1.977(10)
Au2-C28	2.018(10)
N1-C1	1.337(10)
N1-C2	1.390(12)
N1-C4	1.457(10)
N2-C1	1.364(11)
N2-C3	1.391(11)
N2-C16	1.442(10)
N3-C28	1.354(13)
N3-C29	1.366(14)
N3-C31	1.45(2)
N3-C31'	1.46(2)
N4-C28	1.336(13)
N4-C30	1.424(13)
N4-C43	1.451(18)
N4-C43'	1.49(2)
O1-C59	1.347(11)
O1-C60	1.465(13)
O2-C59	1.184(11)
O3-C61	1.321(12)
O3-C62	1.465(11)
O4-C61	1.199(11)
C2-C3	1.354(13)

C2-H2	0.9300
C3-H3	0.9300
C4-C5	1.392(13)
C4-C9	1.392(12)
C5-C6	1.411(13)
C5-C10	1.501(13)
C6-C7	1.344(13)
C6-H6	0.9300
C7-C8	1.420(13)
C7-H7	0.9300
C8-C9	1.393(12)
C8-H8	0.9300
C9-C13	1.513(13)
C10-C11	1.487(17)
C10-C12	1.520(16)
C10-H10	0.9800
C11-H11A	0.9600
C11-H11B	0.9600
C11-H11C	0.9600
C12-H12A	0.9600
C12-H12B	0.9600
C12-H12C	0.9600
C13-C15	1.442(17)
C13-C14	1.499(17)
C13-H13	0.9800
C14-H14A	0.9600
C14-H14B	0.9600
C14-H14C	0.9600
C15-H15A	0.9600
C15-H15B	0.9600
C15-H15C	0.9600
C16-C21	1.379(12)
C16-C17	1.409(12)
C17-C18	1.394(12)
C17-C22	1.509(13)
C18-C19	1.386(13)
C18-H18	0.9300
C19-C20	1.349(13)

C19-H19	0.9300
C20-C21	1.383(11)
C20-H20	0.9300
C21-C25	1.547(13)
C22-C23	1.497(16)
C22-C24	1.509(14)
C22-H22	0.9800
C23-H23A	0.9600
C23-H23B	0.9600
C23-H23C	0.9600
C24-H24A	0.9600
C24-H24B	0.9600
C24-H24C	0.9600
C25-C26	1.541(15)
C25-C27	1.544(15)
C25-H25	0.9800
C26-H26A	0.9600
C26-H26B	0.9600
C26-H26C	0.9600
C27-H27A	0.9600
C27-H27B	0.9600
C27-H27C	0.9600
C29-C30	1.300(17)
C29-H29	0.9300
C30-H30	0.9300
C31-C32	1.389(18)
C31-C36	1.410(19)
C32-C33	1.402(19)
C32-C37	1.49(2)
C33-C34	1.36(2)
C33-H33	0.9300
C34-C35	1.44(2)
C34-H34	0.9300
C35-C36	1.36(2)
C35-H35	0.9300
C36-C40	1.52(2)
C37-C38	1.50(2)
C37-C39	1.61(2)

C37-H37	0.9800
C38-H38A	0.9600
C38-H38B	0.9600
C38-H38C	0.9600
C39-H39A	0.9600
C39-H39B	0.9600
C39-H39C	0.9600
C40-C42	1.51(3)
C40-C41	1.55(3)
C40-H40	0.9800
C41-H41A	0.9600
C41-H41B	0.9600
C41-H41C	0.9600
C42-H42A	0.9600
C42-H42B	0.9600
C42-H42C	0.9600
C31'-C32'	1.389(18)
C31'-C36'	1.41(2)
C32'-C33'	1.401(19)
C32'-C37'	1.49(2)
C33'-C34'	1.36(2)
C33'-H33'	0.9300
C34'-C35'	1.44(2)
C34'-H34'	0.9300
C35'-C36'	1.36(2)
C35'-H35'	0.9300
C36'-C40'	1.52(2)
C37'-C38'	1.50(2)
C37'-C39'	1.61(2)
C37'-H37'	0.9800
C38'-H38D	0.9600
C38'-H38E	0.9600
C38'-H38F	0.9600
C39'-H39D	0.9600
C39'-H39E	0.9600
C39'-H39F	0.9600
C40'-C42'	1.51(3)
C40'-C41'	1.55(3)

C40'-H40'	0.9800
C41'-H41D	0.9600
C41'-H41E	0.9600
C41'-H41F	0.9600
C42'-H42D	0.9600
C42'-H42E	0.9600
C42'-H42F	0.9600
C43-C48	1.381(14)
C43-C44	1.414(14)
C44-C45	1.396(13)
C44-C49	1.504(15)
C45-C46	1.384(16)
C45-H45	0.9300
C46-C47	1.348(15)
C46-H46	0.9300
C47-C48	1.382(13)
C47-H47	0.9300
C48-C52	1.554(15)
C49-C50	1.492(17)
C49-C51	1.507(15)
C49-H49	0.9800
C50-H50A	0.9600
C50-H50B	0.9600
C50-H50C	0.9600
C51-H51A	0.9600
C51-H51B	0.9600
C51-H51C	0.9600
C52-C53	1.551(17)
C52-C54	1.557(17)
C52-H52	0.9800
C53-H53A	0.9600
C53-H53B	0.9600
C53-H53C	0.9600
C54-H54A	0.9600
C54-H54B	0.9600
C54-H54C	0.9600
C43'-C48'	1.383(14)
C43'-C44'	1.412(14)

C44'-C45'	1.396(13)
C44'-C49'	1.510(15)
C45'-C46'	1.384(16)
C45'-H45'	0.9300
C46'-C47'	1.350(15)
C46'-H46'	0.9300
C47'-C48'	1.383(13)
C47'-H47'	0.9300
C48'-C52'	1.554(15)
C49'-C50'	1.496(17)
C49'-C51'	1.512(16)
C49'-H49'	0.9800
C50'-H50D	0.9600
C50'-H50E	0.9600
C50'-H50F	0.9600
C51'-H51D	0.9600
C51'-H51E	0.9600
C51'-H51F	0.9600
C52'-C53'	1.550(17)
C52'-C54'	1.554(17)
C52'-H52'	0.9800
C53'-H53D	0.9600
C53'-H53E	0.9600
C53'-H53F	0.9600
C54'-H54D	0.9600
C54'-H54E	0.9600
C54'-H54F	0.9600
C55-C56	1.237(12)
C56-C57	1.476(12)
C57-C58	1.519(12)
C57-H57A	0.9700
C57-H57B	0.9700
C58-C63	1.520(13)
C58-C61	1.533(12)
C58-C59	1.539(13)
C60-H60A	0.9600
C60-H60B	0.9600
C60-H60C	0.9600

C62-H62A	0.9600
C62-H62B	0.9600
C62-H62C	0.9600
C63-C64	1.503(14)
C63-H63A	0.9700
C63-H63B	0.9700
C64-C65	1.282(14)
C64-H64	0.9300
C65-C66	1.510(15)
C65-C67	1.530(15)
C65-C67'	1.546(18)
C66-H66A	0.9600
C66-H66B	0.9600
C66-H66C	0.9600
C67-H67A	0.9600
C67-H67B	0.9600
C67-H67C	0.9600
C67'-H67D	0.9600
C67'-H67E	0.9600
C67'-H67F	0.9600
B1A-C25A	1.622(14)
B1A-C17A	1.625(12)
B1A-C9A	1.628(11)
B1A-C1A	1.635(12)
B1A-C25"	1.657(15)
C1A-C2A	1.401(13)
C1A-C6A	1.428(14)
C2A-C3A	1.390(14)
C2A-H2A	0.9300
C3A-C4A	1.393(15)
C3A-C7A	1.486(14)
C4A-C5A	1.363(14)
C4A-H4A	0.9300
C5A-C6A	1.387(14)
C5A-C8A	1.508(15)
C6A-H6A	0.9300
C7A-F2'	1.306(14)
C7A-F1A	1.316(14)

C7A-F3'	1.338(13)
C7A-F2A	1.345(13)
C7A-F3A	1.350(14)
C7A-F1'	1.375(14)
C8A-F6'	1.317(14)
C8A-F5A	1.320(14)
C8A-F4A	1.335(16)
C8A-F4'	1.346(16)
C8A-F5'	1.376(15)
C8A-F6A	1.396(14)
C9A-C14A	1.389(13)
C9A-C10A	1.406(13)
C10A-C11A	1.380(15)
C10A-H10A	0.9300
C11A-C12A	1.390(14)
C11A-C15A	1.470(15)
C12A-C13A	1.379(14)
C12A-H12D	0.9300
C13A-C14A	1.387(13)
C13A-C16A	1.474(15)
C14A-H14D	0.9300
C15A-F8'	1.336(15)
C15A-F7A	1.339(15)
C15A-F9A	1.348(15)
C15A-F8A	1.350(15)
C15A-F7'	1.351(15)
C15A-F9'	1.363(15)
C16A-F12'	1.205(19)
C16A-F10A	1.257(17)
C16A-F10'	1.321(17)
C16A-F12A	1.347(19)
C16A-F11A	1.449(16)
C16A-F11'	1.505(18)
C17A-C18A	1.406(13)
C17A-C22A	1.419(13)
C18A-C19A	1.391(14)
C18A-H18A	0.9300
C19A-C20A	1.384(15)

C19A-C23A	1.465(15)
C20A-C21A	1.382(14)
C20A-H20A	0.9300
C21A-C22A	1.378(13)
C21A-C24A	1.474(14)
C22A-H22A	0.9300
C23A-F15A	1.292(15)
C23A-F14'	1.304(15)
C23A-F14A	1.357(13)
C23A-F15'	1.372(15)
C23A-F13'	1.408(14)
C23A-F13A	1.412(15)
C24A-F16A	1.311(14)
C24A-F17A	1.317(13)
C24A-F18'	1.326(15)
C24A-F16'	1.334(14)
C24A-F17'	1.349(14)
C24A-F18A	1.394(13)
C25A-C30A	1.39(2)
C25A-C26A	1.433(17)
C26A-C27A	1.365(17)
C26A-H26D	0.9300
C27A-C28A	1.36(2)
C27A-C31A	1.55(2)
C28A-C29A	1.36(2)
C28A-H28A	0.9300
C29A-C30A	1.409(16)
C29A-C32A	1.461(19)
C30A-H30A	0.9300
C31A-F19A	1.274(19)
C31A-F21A	1.28(2)
C31A-F20A	1.42(2)
C32A-F22A	1.23(9)
C32A-F24A	1.29(7)
C32A-F23A	1.47(5)
C25"-C30"	1.39(2)
C25"-C26"	1.436(18)
C26"-C27"	1.365(17)

C26"-H26"	0.9300
C27"-C28"	1.36(2)
C27"-C31"	1.55(2)
C28"-C29"	1.36(2)
C28"-H28"	0.9300
C29"-C30"	1.410(16)
C29"-C32"	1.460(19)
C30"-H30"	0.9300
C31"-F19"	1.28(2)
C31"-F21"	1.28(2)
C31"-F20"	1.42(2)
C32"-F22"	1.23(9)
C32"-F24"	1.29(7)
C32"-F23"	1.47(5)

Angles----------

C1-Au1-C55	166.8(4)
C1-Au1-C56	160.7(3)
C55-Au1-C56	32.4(3)
C55-Au2-C28	174.4(4)
C1-N1-C2	111.9(7)
C1-N1-C4	124.9(7)
C2-N1-C4	123.0(7)
C1-N2-C3	110.5(7)
C1-N2-C16	124.9(7)
C3-N2-C16	123.6(8)
C28-N3-C29	109.6(10)
C28-N3-C31	127.5(12)
C29-N3-C31	122.1(13)
C28-N3-C31'	124.4(12)
C29-N3-C31'	125.7(11)
C28-N4-C30	109.5(9)
C28-N4-C43	127.4(15)
C30-N4-C43	120.2(16)
C28-N4-C43'	124.6(19)
C30-N4-C43'	126(2)
C59-O1-C60	115.3(8)
C61-O3-C62	115.7(8)

N1-C1-N2	104.8(7)
N1-C1-Au1	129.1(6)
N2-C1-Au1	126.1(6)
C3-C2-N1	106.1(8)
C3-C2-H2	126.9
N1-C2-H2	126.9
C2-C3-N2	106.7(8)
C2-C3-H3	126.7
N2-C3-H3	126.7
C5-C4-C9	124.3(8)
C5-C4-N1	117.6(8)
C9-C4-N1	118.1(8)
C4-C5-C6	116.2(9)
C4-C5-C10	124.4(8)
C6-C5-C10	119.3(9)
C7-C6-C5	121.6(9)
C7-C6-H6	119.2
C5-C6-H6	119.2
C6-C7-C8	120.9(9)
C6-C7-H7	119.5
C8-C7-H7	119.5
C9-C8-C7	119.8(9)
C9-C8-H8	120.1
C7-C8-H8	120.1
C4-C9-C8	117.1(8)
C4-C9-C13	124.2(8)
C8-C9-C13	118.7(8)
C11-C10-C5	114.2(10)
C11-C10-C12	110.6(10)
C5-C10-C12	111.3(10)
C11-C10-H10	106.8
C5-C10-H10	106.8
C12-C10-H10	106.8
C10-C11-H11A	109.5
C10-C11-H11B	109.5
H11A-C11-H11B	109.5
C10-C11-H11C	109.5
H11A-C11-H11C	109.5

H11B-C11-H11C	109.5
C10-C12-H12A	109.5
C10-C12-H12B	109.5
H12A-C12-H12B	109.5
C10-C12-H12C	109.5
H12A-C12-H12C	109.5
H12B-C12-H12C	109.5
C15-C13-C14	114.0(13)
C15-C13-C9	112.5(10)
C14-C13-C9	110.0(10)
C15-C13-H13	106.6
C14-C13-H13	106.6
C9-C13-H13	106.6
C13-C14-H14A	109.5
C13-C14-H14B	109.5
H14A-C14-H14B	109.5
C13-C14-H14C	109.5
H14A-C14-H14C	109.5
H14B-C14-H14C	109.5
C13-C15-H15A	109.5
C13-C15-H15B	109.5
H15A-C15-H15B	109.5
C13-C15-H15C	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.5
C21-C16-C17	123.1(8)
C21-C16-N2	118.6(8)
C17-C16-N2	118.3(8)
C18-C17-C16	115.1(8)
C18-C17-C22	122.4(9)
C16-C17-C22	122.5(8)
C19-C18-C17	122.3(9)
C19-C18-H18	118.9
C17-C18-H18	118.9
C20-C19-C18	120.2(8)
C20-C19-H19	119.9
C18-C19-H19	119.9
C19-C20-C21	120.8(9)

C19-C20-H20	119.6
C21-C20-H20	119.6
C16-C21-C20	118.5(9)
C16-C21-C25	122.5(8)
C20-C21-C25	118.8(8)
C23-C22-C17	108.6(9)
C23-C22-C24	109.8(10)
C17-C22-C24	112.9(8)
C23-C22-H22	108.5
C17-C22-H22	108.5
C24-C22-H22	108.5
C22-C23-H23A	109.5
C22-C23-H23B	109.5
H23A-C23-H23B	109.5
C22-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C22-C24-H24A	109.5
C22-C24-H24B	109.5
H24A-C24-H24B	109.5
C22-C24-H24C	109.5
H24A-C24-H24C	109.5
H24B-C24-H24C	109.5
C26-C25-C27	111.6(9)
C26-C25-C21	110.5(9)
C27-C25-C21	111.5(9)
C26-C25-H25	107.7
C27-C25-H25	107.7
C21-C25-H25	107.7
C25-C26-H26A	109.5
C25-C26-H26B	109.5
H26A-C26-H26B	109.5
C25-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C25-C27-H27A	109.5
C25-C27-H27B	109.5
H27A-C27-H27B	109.5

C25-C27-H27C	109.5
H27A-C27-H27C	109.5
H27B-C27-H27C	109.5
N4-C28-N3	105.6(9)
N4-C28-Au2	125.0(7)
N3-C28-Au2	128.9(8)
C30-C29-N3	109.5(10)
C30-C29-H29	125.3
N3-C29-H29	125.3
C29-C30-N4	105.8(10)
C29-C30-H30	127.1
N4-C30-H30	127.1
C32-C31-C36	123.5(14)
C32-C31-N3	120.6(15)
C36-C31-N3	115.9(15)
C31-C32-C33	117.5(15)
C31-C32-C37	123.1(14)
C33-C32-C37	119.1(15)
C34-C33-C32	119.7(16)
C34-C33-H33	120.2
C32-C33-H33	120.2
C33-C34-C35	122.0(16)
C33-C34-H34	119.0
C35-C34-H34	119.0
C36-C35-C34	118.5(17)
C36-C35-H35	120.7
C34-C35-H35	120.7
C35-C36-C31	118.3(16)
C35-C36-C40	119.2(17)
C31-C36-C40	122.3(16)
C32-C37-C38	114.5(17)
C32-C37-C39	111.6(15)
C38-C37-C39	106.9(15)
C32-C37-H37	107.9
C38-C37-H37	107.9
C39-C37-H37	107.9
C37-C38-H38A	109.5
C37-C38-H38B	109.5

H38A-C38-H38B	109.5
C37-C38-H38C	109.5
H38A-C38-H38C	109.5
H38B-C38-H38C	109.5
C37-C39-H39A	109.5
C37-C39-H39B	109.5
H39A-C39-H39B	109.5
C37-C39-H39C	109.5
H39A-C39-H39C	109.5
H39B-C39-H39C	109.5
C42-C40-C36	110.9(17)
C42-C40-C41	111.8(19)
C36-C40-C41	110.2(19)
C42-C40-H40	107.9
C36-C40-H40	107.9
C41-C40-H40	107.9
C40-C41-H41A	109.5
C40-C41-H41B	109.5
H41A-C41-H41B	109.5
C40-C41-H41C	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
C40-C42-H42A	109.5
C40-C42-H42B	109.5
H42A-C42-H42B	109.5
C40-C42-H42C	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
C32'-C31'-C36'	123.8(14)
C32'-C31'-N3	114.5(17)
C36'-C31'-N3	121.2(15)
C31'-C32'-C33'	117.5(16)
C31'-C32'-C37'	122.9(15)
C33'-C32'-C37'	119.6(16)
C34'-C33'-C32'	119.7(17)
C34'-C33'-H33'	120.1
C32'-C33'-H33'	120.1
C33'-C34'-C35'	122.3(17)

C33'-C34'-H34'	118.9
C35'-C34'-H34'	118.9
C36'-C35'-C34'	118.5(18)
C36'-C35'-H35'	120.8
C34'-C35'-H35'	120.8
C35'-C36'-C31'	118.0(17)
C35'-C36'-C40'	119.7(18)
C31'-C36'-C40'	122.2(16)
C32'-C37'-C38'	115.6(18)
C32'-C37'-C39'	112.2(17)
C38'-C37'-C39'	107.1(16)
C32'-C37'-H37'	107.2
C38'-C37'-H37'	107.2
C39'-C37'-H37'	107.2
C37'-C38'-H38D	109.5
C37'-C38'-H38E	109.5
H38D-C38'-H38E	109.5
C37'-C38'-H38F	109.5
H38D-C38'-H38F	109.5
H38E-C38'-H38F	109.5
C37'-C39'-H39D	109.5
C37'-C39'-H39E	109.5
H39D-C39'-H39E	109.5
C37'-C39'-H39F	109.5
H39D-C39'-H39F	109.5
H39E-C39'-H39F	109.5
C42'-C40'-C36'	111.4(17)
C42'-C40'-C41'	112(2)
C36'-C40'-C41'	111(2)
C42'-C40'-H40'	107.4
C36'-C40'-H40'	107.4
C41'-C40'-H40'	107.4
C40'-C41'-H41D	109.5
C40'-C41'-H41E	109.5
H41D-C41'-H41E	109.5
C40'-C41'-H41F	109.5
H41D-C41'-H41F	109.5
H41E-C41'-H41F	109.5

C40'-C42'-H42D	109.5
C40'-C42'-H42E	109.5
H42D-C42'-H42E	109.5
C40'-C42'-H42F	109.5
H42D-C42'-H42F	109.5
H42E-C42'-H42F	109.5
C48-C43-C44	123.2(11)
C48-C43-N4	112.7(13)
C44-C43-N4	124.0(13)
C45-C44-C43	114.5(12)
C45-C44-C49	122.2(13)
C43-C44-C49	123.3(11)
C46-C45-C44	122.2(13)
C46-C45-H45	118.9
C44-C45-H45	118.9
C47-C46-C45	120.6(13)
C47-C46-H46	119.7
C45-C46-H46	119.7
C46-C47-C48	120.6(13)
C46-C47-H47	119.7
C48-C47-H47	119.7
C43-C48-C47	118.2(12)
C43-C48-C52	123.2(11)
C47-C48-C52	118.3(12)
C50-C49-C44	111.4(13)
C50-C49-C51	109.6(14)
C44-C49-C51	114.0(14)
C50-C49-H49	107.2
C44-C49-H49	107.2
C51-C49-H49	107.2
C49-C50-H50A	109.5
C49-C50-H50B	109.5
H50A-C50-H50B	109.5
C49-C50-H50C	109.5
H50A-C50-H50C	109.5
H50B-C50-H50C	109.5
C49-C51-H51A	109.5
C49-C51-H51B	109.5

H51A-C51-H51B	109.5
C49-C51-H51C	109.5
H51A-C51-H51C	109.5
H51B-C51-H51C	109.5
C53-C52-C48	109.1(13)
C53-C52-C54	108.9(13)
C48-C52-C54	108.6(13)
C53-C52-H52	110.0
C48-C52-H52	110.0
C54-C52-H52	110.0
C52-C53-H53A	109.5
C52-C53-H53B	109.5
H53A-C53-H53B	109.5
C52-C53-H53C	109.5
H53A-C53-H53C	109.5
H53B-C53-H53C	109.5
C52-C54-H54A	109.5
C52-C54-H54B	109.5
H54A-C54-H54B	109.5
C52-C54-H54C	109.5
H54A-C54-H54C	109.5
H54B-C54-H54C	109.5
C48'-C43'-C44'	123.1(12)
C48'-C43'-N4	122.9(15)
C44'-C43'-N4	113.4(14)
C45'-C44'-C43'	114.3(12)
C45'-C44'-C49'	121.3(13)
C43'-C44'-C49'	123.7(12)
C46'-C45'-C44'	122.5(13)
C46'-C45'-H45'	118.8
C44'-C45'-H45'	118.8
C47'-C46'-C45'	120.6(13)
C47'-C46'-H46'	119.7
C45'-C46'-H46'	119.7
C46'-C47'-C48'	120.1(13)
C46'-C47'-H47'	120.0
C48'-C47'-H47'	120.0
C47'-C48'-C43'	118.9(13)

C47'-C48'-C52'	118.7(13)
C43'-C48'-C52'	122.3(12)
C50'-C49'-C44'	109.2(14)
C50'-C49'-C51'	108.6(14)
C44'-C49'-C51'	113.0(15)
C50'-C49'-H49'	108.7
C44'-C49'-H49'	108.7
C51'-C49'-H49'	108.7
C49'-C50'-H50D	109.5
C49'-C50'-H50E	109.5
H50D-C50'-H50E	109.5
C49'-C50'-H50F	109.5
H50D-C50'-H50F	109.5
H50E-C50'-H50F	109.5
C49'-C51'-H51D	109.5
C49'-C51'-H51E	109.5
H51D-C51'-H51E	109.5
C49'-C51'-H51F	109.5
H51D-C51'-H51F	109.5
H51E-C51'-H51F	109.5
C53'-C52'-C48'	109.3(14)
C53'-C52'-C54'	109.6(14)
C48'-C52'-C54'	108.9(14)
C53'-C52'-H52'	109.7
C48'-C52'-H52'	109.7
C54'-C52'-H52'	109.7
C52'-C53'-H53D	109.5
C52'-C53'-H53E	109.5
H53D-C53'-H53E	109.5
C52'-C53'-H53F	109.5
H53D-C53'-H53F	109.5
H53E-C53'-H53F	109.5
C52'-C54'-H54D	109.5
C52'-C54'-H54E	109.5
H54D-C54'-H54E	109.5
C52'-C54'-H54F	109.5
H54D-C54'-H54F	109.5
H54E-C54'-H54F	109.5

C56-C55-Au2	172.5(8)
C56-C55-Au1	74.6(6)
Au2-C55-Au1	112.8(4)
C55-C56-C57	166.1(9)
C55-C56-Au1	73.0(6)
C57-C56-Au1	119.8(6)
C56-C57-C58	113.6(7)
C56-C57-H57A	108.8
C58-C57-H57A	108.8
C56-C57-H57B	108.8
C58-C57-H57B	108.8
H57A-C57-H57B	107.7
C57-C58-C63	113.4(8)
C57-C58-C61	108.6(7)
C63-C58-C61	109.4(8)
C57-C58-C59	106.8(7)
C63-C58-C59	110.3(8)
C61-C58-C59	108.2(7)
O2-C59-O1	123.5(9)
O2-C59-C58	125.3(9)
O1-C59-C58	111.2(8)
O1-C60-H60A	109.5
O1-C60-H60B	109.5
H60A-C60-H60B	109.5
O1-C60-H60C	109.5
H60A-C60-H60C	109.5
H60B-C60-H60C	109.5
O4-C61-O3	125.0(9)
O4-C61-C58	123.2(9)
O3-C61-C58	111.7(8)
O3-C62-H62A	109.5
O3-C62-H62B	109.5
H62A-C62-H62B	109.5
O3-C62-H62C	109.5
H62A-C62-H62C	109.5
H62B-C62-H62C	109.5
C64-C63-C58	114.2(8)
C64-C63-H63A	108.7

C58-C63-H63A	108.7
C64-C63-H63B	108.7
C58-C63-H63B	108.7
H63A-C63-H63B	107.6
C65-C64-C63	129.7(10)
C65-C64-H64	115.2
C63-C64-H64	115.2
C64-C65-C66	122.2(10)
C64-C65-C67	124.6(14)
C66-C65-C67	112.3(14)
C64-C65-C67'	114.1(19)
C66-C65-C67'	119(2)
C65-C66-H66A	109.5
C65-C66-H66B	109.5
H66A-C66-H66B	109.5
C65-C66-H66C	109.5
H66A-C66-H66C	109.5
H66B-C66-H66C	109.5
C65-C67-H67A	109.5
C65-C67-H67B	109.5
H67A-C67-H67B	109.5
C65-C67-H67C	109.5
H67A-C67-H67C	109.5
H67B-C67-H67C	109.5
C65-C67'-H67D	109.5
C65-C67'-H67E	109.5
H67D-C67'-H67E	109.5
C65-C67'-H67F	109.5
H67D-C67'-H67F	109.5
H67E-C67'-H67F	109.5
C25A-B1A-C17A	107.7(8)
C25A-B1A-C9A	108.0(7)
C17A-B1A-C9A	113.5(7)
C25A-B1A-C1A	111.1(9)
C17A-B1A-C1A	104.7(7)
C9A-B1A-C1A	111.8(7)
C17A-B1A-C25"	114.9(8)
C9A-B1A-C25"	99.4(7)

C1A-B1A-C25"	113.0(10)
C2A-C1A-C6A	114.3(9)
C2A-C1A-B1A	122.7(8)
C6A-C1A-B1A	122.9(8)
C3A-C2A-C1A	123.9(10)
C3A-C2A-H2A	118.1
C1A-C2A-H2A	118.1
C2A-C3A-C4A	119.9(10)
C2A-C3A-C7A	121.4(10)
C4A-C3A-C7A	118.7(10)
C5A-C4A-C3A	118.0(10)
C5A-C4A-H4A	121.0
C3A-C4A-H4A	121.0
C4A-C5A-C6A	122.7(10)
C4A-C5A-C8A	121.2(10)
C6A-C5A-C8A	116.0(9)
C5A-C6A-C1A	121.2(9)
C5A-C6A-H6A	119.4
C1A-C6A-H6A	119.4
F2'-C7A-F3'	108.9(13)
F1A-C7A-F2A	108.0(12)
F1A-C7A-F3A	106.8(12)
F2A-C7A-F3A	104.8(11)
F2'-C7A-F1'	104.8(12)
F3'-C7A-F1'	102.2(11)
F2'-C7A-C3A	116.3(15)
F1A-C7A-C3A	114.0(13)
F3'-C7A-C3A	114.2(11)
F2A-C7A-C3A	110.5(10)
F3A-C7A-C3A	112.1(13)
F1'-C7A-C3A	109.1(12)
F5A-C8A-F4A	109.7(15)
F6'-C8A-F4'	108.0(15)
F6'-C8A-F5'	106.1(12)
F4'-C8A-F5'	104.3(14)
F5A-C8A-F6A	102.8(11)
F4A-C8A-F6A	104.4(14)
F6'-C8A-C5A	118.9(14)

F5A-C8A-C5A	117.8(12)
F4A-C8A-C5A	114.3(19)
F4'-C8A-C5A	112.3(19)
F5'-C8A-C5A	106.0(12)
F6A-C8A-C5A	106.3(12)
C14A-C9A-C10A	114.4(8)
C14A-C9A-B1A	123.7(8)
C10A-C9A-B1A	121.5(8)
C11A-C10A-C9A	123.5(9)
C11A-C10A-H10A	118.2
C9A-C10A-H10A	118.2
C10A-C11A-C12A	119.8(10)
C10A-C11A-C15A	120.5(9)
C12A-C11A-C15A	119.7(10)
C13A-C12A-C11A	118.4(10)
C13A-C12A-H12D	120.8
C11A-C12A-H12D	120.8
C12A-C13A-C14A	120.6(9)
C12A-C13A-C16A	119.9(10)
C14A-C13A-C16A	119.5(9)
C13A-C14A-C9A	123.1(9)
C13A-C14A-H14D	118.4
C9A-C14A-H14D	118.4
F7A-C15A-F9A	108.3(14)
F7A-C15A-F8A	105.5(13)
F9A-C15A-F8A	103.8(13)
F8'-C15A-F7'	103.9(14)
F8'-C15A-F9'	107.4(14)
F7'-C15A-F9'	103.8(14)
F8'-C15A-C11A	113.3(17)
F7A-C15A-C11A	110.3(15)
F9A-C15A-C11A	114.9(15)
F8A-C15A-C11A	113.3(13)
F7'-C15A-C11A	114.2(16)
F9'-C15A-C11A	113.4(14)
F12'-C16A-F10'	116.3(15)
F10A-C16A-F12A	109.4(15)
F10A-C16A-F11A	104.9(13)

F12A-C16A-F11A	99.6(12)
F12'-C16A-C13A	117.8(16)
F10A-C16A-C13A	118.8(13)
F10'-C16A-C13A	113.6(12)
F12A-C16A-C13A	112.7(12)
F11A-C16A-C13A	109.4(10)
F12'-C16A-F11'	103.3(13)
F10'-C16A-F11'	95.9(12)
C13A-C16A-F11'	106.2(11)
C18A-C17A-C22A	113.4(8)
C18A-C17A-B1A	124.4(8)
C22A-C17A-B1A	122.2(8)
C19A-C18A-C17A	123.4(9)
C19A-C18A-H18A	118.3
C17A-C18A-H18A	118.3
C20A-C19A-C18A	120.8(10)
C20A-C19A-C23A	120.1(10)
C18A-C19A-C23A	119.1(10)
C21A-C20A-C19A	117.9(10)
C21A-C20A-H20A	121.1
C19A-C20A-H20A	121.1
C22A-C21A-C20A	121.0(10)
C22A-C21A-C24A	119.6(9)
C20A-C21A-C24A	119.3(9)
C21A-C22A-C17A	123.5(9)
C21A-C22A-H22A	118.2
C17A-C22A-H22A	118.2
F15A-C23A-F14A	110.7(14)
F14'-C23A-F15'	104.7(15)
F14'-C23A-F13'	107.0(12)
F15'-C23A-F13'	99.9(13)
F15A-C23A-F13A	105.7(14)
F14A-C23A-F13A	100.5(11)
F15A-C23A-C19A	117.9(17)
F14'-C23A-C19A	121.0(15)
F14A-C23A-C19A	113.3(11)
F15'-C23A-C19A	112.1(16)
F13'-C23A-C19A	110.0(13)

F13A-C23A-C19A	106.8(12)
F16A-C24A-F17A	110.4(13)
F18'-C24A-F16'	104.3(13)
F18'-C24A-F17'	106.9(13)
F16'-C24A-F17'	105.8(12)
F16A-C24A-F18A	105.2(11)
F17A-C24A-F18A	100.4(10)
F16A-C24A-C21A	115.8(13)
F17A-C24A-C21A	113.6(11)
F18'-C24A-C21A	114.5(14)
F16'-C24A-C21A	109.3(12)
F17'-C24A-C21A	115.2(14)
F18A-C24A-C21A	110.0(10)
C30A-C25A-C26A	113.5(15)
C30A-C25A-B1A	125.9(15)
C26A-C25A-B1A	116.3(13)
C27A-C26A-C25A	120.5(14)
C27A-C26A-H26D	119.7
C25A-C26A-H26D	119.7
C28A-C27A-C26A	122.7(15)
C28A-C27A-C31A	120.4(15)
C26A-C27A-C31A	116.1(15)
C29A-C28A-C27A	117.6(18)
C29A-C28A-H28A	121.2
C27A-C28A-H28A	121.2
C28A-C29A-C30A	120.4(14)
C28A-C29A-C32A	119.5(12)
C30A-C29A-C32A	120.0(12)
C25A-C30A-C29A	121.9(16)
C25A-C30A-H30A	119.0
C29A-C30A-H30A	119.0
F19A-C31A-F21A	111.5(19)
F19A-C31A-F20A	105.2(18)
F21A-C31A-F20A	100(2)
F19A-C31A-C27A	113.7(18)
F21A-C31A-C27A	115.6(17)
F20A-C31A-C27A	109.2(16)
F22A-C32A-F24A	114(3)

F22A-C32A-C29A	115(6)
F24A-C32A-C29A	115(4)
F22A-C32A-F23A	100(3)
F24A-C32A-F23A	97(5)
C29A-C32A-F23A	111(2)
C30"-C25"-C26"	113.1(16)
C30"-C25"-B1A	127.0(18)
C26"-C25"-B1A	115.5(14)
C27"-C26"-C25"	120.5(15)
C27"-C26"-H26"	119.7
C25"-C26"-H26"	119.7
C28"-C27"-C26"	122.3(15)
C28"-C27"-C31"	120.0(16)
C26"-C27"-C31"	116.8(16)
C29"-C28"-C27"	118.1(19)
C29"-C28"-H28"	121.0
C27"-C28"-H28"	121.0
C28"-C29"-C30"	119.8(14)
C28"-C29"-C32"	119.7(12)
C30"-C29"-C32"	120.4(13)
C25"-C30"-C29"	122.3(17)
C25"-C30"-H30"	118.8
C29"-C30"-H30"	118.8
F19"-C31"-F21"	111.2(19)
F19"-C31"-F20"	104.9(18)
F21"-C31"-F20"	100(2)
F19"-C31"-C27"	112.7(18)
F21"-C31"-C27"	116.9(16)
F20"-C31"-C27"	109.5(17)
F22"-C32"-F24"	113(3)
F22"-C32"-C29"	116(6)
F24"-C32"-C29"	115(5)
F22"-C32"-F23"	100(3)
F24"-C32"-F23"	96(5)
C29"-C32"-F23"	113(3)

Table 3. Torsion angles [°] for SCF-A-14_twin1_hklf5.

C2-N1-C1-N2	0.7(10)
C4-N1-C1-N2	175.1(8)
C2-N1-C1-Au1	-179.8(7)
C4-N1-C1-Au1	-5.3(13)
C3-N2-C1-N1	-1.3(10)
C16-N2-C1-N1	-170.7(8)
C3-N2-C1-Au1	179.1(7)
C16-N2-C1-Au1	9.7(12)
C1-N1-C2-C3	0.2(11)
C4-N1-C2-C3	-174.4(9)
N1-C2-C3-N2	-1.0(11)
C1-N2-C3-C2	1.4(11)
C16-N2-C3-C2	171.0(9)
C1-N1-C4-C5	-87.4(11)
C2-N1-C4-C5	86.5(11)
C1-N1-C4-C9	94.9(10)
C2-N1-C4-C9	-91.3(11)
C9-C4-C5-C6	-1.4(14)
N1-C4-C5-C6	-179.0(8)
C9-C4-C5-C10	-179.6(9)
N1-C4-C5-C10	2.8(14)
C4-C5-C6-C7	1.1(14)
C10-C5-C6-C7	179.4(10)
C5-C6-C7-C8	0.2(15)
C6-C7-C8-C9	-1.3(14)
C5-C4-C9-C8	0.4(13)
N1-C4-C9-C8	178.0(8)
C5-C4-C9-C13	-178.5(9)
N1-C4-C9-C13	-1.0(13)
C7-C8-C9-C4	1.0(13)
C7-C8-C9-C13	180.0(9)
C4-C5-C10-C11	-123.0(13)
C6-C5-C10-C11	58.9(15)
C4-C5-C10-C12	111.0(12)
C6-C5-C10-C12	-67.1(13)
C4-C9-C13-C15	-121.4(13)
C8-C9-C13-C15	59.7(14)
C4-C9-C13-C14	110.3(11)

C8-C9-C13-C14	-68.6(13)
C1-N2-C16-C21	77.7(12)
C3-N2-C16-C21	-90.4(11)
C1-N2-C16-C17	-102.0(11)
C3-N2-C16-C17	89.9(11)
C21-C16-C17-C18	2.3(14)
N2-C16-C17-C18	-178.0(9)
C21-C16-C17-C22	-175.8(9)
N2-C16-C17-C22	4.0(14)
C16-C17-C18-C19	0.4(15)
C22-C17-C18-C19	178.4(10)
C17-C18-C19-C20	-3.3(16)
C18-C19-C20-C21	3.7(16)
C17-C16-C21-C20	-2.0(15)
N2-C16-C21-C20	178.3(9)
C17-C16-C21-C25	173.0(9)
N2-C16-C21-C25	-6.7(14)
C19-C20-C21-C16	-1.1(15)
C19-C20-C21-C25	-176.3(10)
C18-C17-C22-C23	-80.4(14)
C16-C17-C22-C23	97.5(13)
C18-C17-C22-C24	41.7(14)
C16-C17-C22-C24	-140.4(10)
C16-C21-C25-C26	-112.7(10)
C20-C21-C25-C26	62.3(12)
C16-C21-C25-C27	122.5(11)
C20-C21-C25-C27	-62.5(13)
C30-N4-C28-N3	0.5(15)
C43-N4-C28-N3	161.0(15)
C43'-N4-C28-N3	-174.3(14)
C30-N4-C28-Au2	-171.7(10)
C43-N4-C28-Au2	-11(2)
C43'-N4-C28-Au2	13(2)
C29-N3-C28-N4	-0.7(15)
C31-N3-C28-N4	-170.2(14)
C31'-N3-C28-N4	-175.1(13)
C29-N3-C28-Au2	171.2(10)
C31-N3-C28-Au2	2(2)

C31'-N3-C28-Au2	-3.2(19)
C28-N3-C29-C30	0.6(18)
C31-N3-C29-C30	170.7(15)
C31'-N3-C29-C30	174.9(15)
N3-C29-C30-N4	-0.2(18)
C28-N4-C30-C29	-0.2(17)
C43-N4-C30-C29	-162.4(14)
C43'-N4-C30-C29	174.6(16)
C28-N3-C31-C32	-104(3)
C29-N3-C31-C32	88(3)
C28-N3-C31-C36	77(3)
C29-N3-C31-C36	-91(2)
C36-C31-C32-C33	3(5)
N3-C31-C32-C33	-176(3)
C36-C31-C32-C37	176(3)
N3-C31-C32-C37	-3(4)
C31-C32-C33-C34	-7(5)
C37-C32-C33-C34	-180(3)
C32-C33-C34-C35	8(5)
C33-C34-C35-C36	-6(5)
C34-C35-C36-C31	2(5)
C34-C35-C36-C40	177(3)
C32-C31-C36-C35	-1(5)
N3-C31-C36-C35	178(3)
C32-C31-C36-C40	-176(3)
N3-C31-C36-C40	3(3)
C31-C32-C37-C38	140(3)
C33-C32-C37-C38	-47(3)
C31-C32-C37-C39	-98(4)
C33-C32-C37-C39	74(3)
C35-C36-C40-C42	-69(3)
C31-C36-C40-C42	106(3)
C35-C36-C40-C41	56(3)
C31-C36-C40-C41	-130(3)
C28-N3-C31'-C32'	-107(3)
C29-N3-C31'-C32'	79(3)
C28-N3-C31'-C36'	81(2)
C29-N3-C31'-C36'	-92(3)

C36'-C31'-C32'-C33'	-2(6)
N3-C31'-C32'-C33'	-174(3)
C36'-C31'-C32'-C37'	-180(3)
N3-C31'-C32'-C37'	9(4)
C31'-C32'-C33'-C34'	1(6)
C37'-C32'-C33'-C34'	179(3)
C32'-C33'-C34'-C35'	-3(6)
C33'-C34'-C35'-C36'	5(6)
C34'-C35'-C36'-C31'	-5(6)
C34'-C35'-C36'-C40'	177(3)
C32'-C31'-C36'-C35'	4(6)
N3-C31'-C36'-C35'	175(3)
C32'-C31'-C36'-C40'	-178(3)
N3-C31'-C36'-C40'	-7(4)
C31'-C32'-C37'-C38'	136(4)
C33'-C32'-C37'-C38'	-42(4)
C31'-C32'-C37'-C39'	-101(4)
C33'-C32'-C37'-C39'	82(4)
C35'-C36'-C40'-C42'	-60(4)
C31'-C36'-C40'-C42'	123(4)
C35'-C36'-C40'-C41'	66(4)
C31'-C36'-C40'-C41'	-111(4)
C28-N4-C43-C48	114(2)
C30-N4-C43-C48	-88(3)
C28-N4-C43-C44	-63(4)
C30-N4-C43-C44	96(3)
C48-C43-C44-C45	6(4)
N4-C43-C44-C45	-178(3)
C48-C43-C44-C49	-176(2)
N4-C43-C44-C49	0(4)
C43-C44-C45-C46	1(4)
C49-C44-C45-C46	-177(2)
C44-C45-C46-C47	-4(4)
C45-C46-C47-C48	0(4)
C44-C43-C48-C47	-10(4)
N4-C43-C48-C47	174(2)
C44-C43-C48-C52	176(2)
N4-C43-C48-C52	0(4)

C46-C47-C48-C43	6(4)
C46-C47-C48-C52	-179(2)
C45-C44-C49-C50	-35(3)
C43-C44-C49-C50	148(3)
C45-C44-C49-C51	90(3)
C43-C44-C49-C51	-88(3)
C43-C48-C52-C53	112(3)
C47-C48-C52-C53	-62(2)
C43-C48-C52-C54	-129(3)
C47-C48-C52-C54	57(3)
C28-N4-C43'-C48'	96(4)
C30-N4-C43'-C48'	-78(4)
C28-N4-C43'-C44'	-93(3)
C30-N4-C43'-C44'	93(3)
C48'-C43'-C44'-C45'	-7(5)
N4-C43'-C44'-C45'	-179(3)
C48'-C43'-C44'-C49'	-178(3)
N4-C43'-C44'-C49'	11(4)
C43'-C44'-C45'-C46'	8(5)
C49'-C44'-C45'-C46'	179(3)
C44'-C45'-C46'-C47'	-3(5)
C45'-C46'-C47'-C48'	-4(5)
C46'-C47'-C48'-C43'	5(5)
C46'-C47'-C48'-C52'	-179(3)
C44'-C43'-C48'-C47'	1(5)
N4-C43'-C48'-C47'	172(3)
C44'-C43'-C48'-C52'	-175(3)
N4-C43'-C48'-C52'	-4(5)
C45'-C44'-C49'-C50'	-52(3)
C43'-C44'-C49'-C50'	118(3)
C45'-C44'-C49'-C51'	69(3)
C43'-C44'-C49'-C51'	-121(3)
C47'-C48'-C52'-C53'	51(3)
C43'-C48'-C52'-C53'	-133(3)
C47'-C48'-C52'-C54'	-68(3)
C43'-C48'-C52'-C54'	107(3)
Au1-C55-C56-C57	-158(4)
C55-C56-C57-C58	-34(4)

Au1-C56-C57-C58	170.0(6)
C56-C57-C58-C63	45.4(10)
C56-C57-C58-C61	-76.5(9)
C56-C57-C58-C59	167.1(7)
C60-O1-C59-O2	1.0(14)
C60-O1-C59-C58	-178.4(9)
C57-C58-C59-O2	0.8(13)
C63-C58-C59-O2	124.5(10)
C61-C58-C59-O2	-115.9(11)
C57-C58-C59-O1	-179.8(7)
C63-C58-C59-O1	-56.1(10)
C61-C58-C59-O1	63.5(10)
C62-O3-C61-O4	1.4(15)
C62-O3-C61-C58	177.6(8)
C57-C58-C61-O4	97.3(11)
C63-C58-C61-O4	-26.9(13)
C59-C58-C61-O4	-147.2(10)
C57-C58-C61-O3	-79.0(10)
C63-C58-C61-O3	156.7(8)
C59-C58-C61-O3	36.5(11)
C57-C58-C63-C64	61.2(11)
C61-C58-C63-C64	-177.5(9)
C59-C58-C63-C64	-58.6(11)
C58-C63-C64-C65	138.9(13)
C63-C64-C65-C66	177.7(11)
C63-C64-C65-C67	10(2)
C63-C64-C65-C67'	-28(3)
C25A-B1A-C1A-C2A	-41.1(12)
C17A-B1A-C1A-C2A	74.9(11)
C9A-B1A-C1A-C2A	-161.8(9)
C25"-B1A-C1A-C2A	-50.7(11)
C25A-B1A-C1A-C6A	142.0(9)
C17A-B1A-C1A-C6A	-102.0(10)
C9A-B1A-C1A-C6A	21.2(12)
C25"-B1A-C1A-C6A	132.3(9)
C6A-C1A-C2A-C3A	1.2(15)
B1A-C1A-C2A-C3A	-176.0(9)
C1A-C2A-C3A-C4A	-2.5(16)

C1A-C2A-C3A-C7A	176.7(9)
C2A-C3A-C4A-C5A	2.2(16)
C7A-C3A-C4A-C5A	-177.1(10)
C3A-C4A-C5A-C6A	-0.7(17)
C3A-C4A-C5A-C8A	179.5(10)
C4A-C5A-C6A-C1A	-0.6(17)
C8A-C5A-C6A-C1A	179.2(10)
C2A-C1A-C6A-C5A	0.4(15)
B1A-C1A-C6A-C5A	177.6(9)
C2A-C3A-C7A-F2'	134.3(13)
C4A-C3A-C7A-F2'	-46.5(16)
C2A-C3A-C7A-F1A	-80.1(14)
C4A-C3A-C7A-F1A	99.2(14)
C2A-C3A-C7A-F3'	6.1(16)
C4A-C3A-C7A-F3'	-174.6(12)
C2A-C3A-C7A-F2A	41.8(14)
C4A-C3A-C7A-F2A	-138.9(11)
C2A-C3A-C7A-F3A	158.4(12)
C4A-C3A-C7A-F3A	-22.4(15)
C2A-C3A-C7A-F1'	-107.5(13)
C4A-C3A-C7A-F1'	71.8(14)
C4A-C5A-C8A-F6'	127.1(15)
C6A-C5A-C8A-F6'	-52.7(17)
C4A-C5A-C8A-F5A	-146.5(14)
C6A-C5A-C8A-F5A	33.7(17)
C4A-C5A-C8A-F4A	-15.5(19)
C6A-C5A-C8A-F4A	164.6(15)
C4A-C5A-C8A-F4'	-0.3(19)
C6A-C5A-C8A-F4'	179.9(15)
C4A-C5A-C8A-F5'	-113.6(14)
C6A-C5A-C8A-F5'	66.6(14)
C4A-C5A-C8A-F6A	99.1(14)
C6A-C5A-C8A-F6A	-80.8(13)
C25A-B1A-C9A-C14A	96.9(12)
C17A-B1A-C9A-C14A	-22.5(13)
C1A-B1A-C9A-C14A	-140.6(9)
C25"-B1A-C9A-C14A	99.9(12)
C25A-B1A-C9A-C10A	-75.3(13)

C17A-B1A-C9A-C10A	165.3(10)
C1A-B1A-C9A-C10A	47.3(12)
C25"-B1A-C9A-C10A	-72.2(13)
C14A-C9A-C10A-C11A	3.9(17)
B1A-C9A-C10A-C11A	176.7(11)
C9A-C10A-C11A-C12A	-2(2)
C9A-C10A-C11A-C15A	179.2(11)
C10A-C11A-C12A-C13A	-1.2(19)
C15A-C11A-C12A-C13A	178.0(12)
C11A-C12A-C13A-C14A	1.4(18)
C11A-C12A-C13A-C16A	-177.2(12)
C12A-C13A-C14A-C9A	1.2(17)
C16A-C13A-C14A-C9A	179.8(10)
C10A-C9A-C14A-C13A	-3.7(15)
B1A-C9A-C14A-C13A	-176.4(9)
C10A-C11A-C15A-F8'	79.3(17)
C12A-C11A-C15A-F8'	-99.9(16)
C10A-C11A-C15A-F7A	-62.1(17)
C12A-C11A-C15A-F7A	118.7(15)
C10A-C11A-C15A-F9A	175.1(15)
C12A-C11A-C15A-F9A	-4(2)
C10A-C11A-C15A-F8A	55.9(17)
C12A-C11A-C15A-F8A	-123.3(14)
C10A-C11A-C15A-F7'	-39(2)
C12A-C11A-C15A-F7'	141.5(15)
C10A-C11A-C15A-F9'	-157.9(14)
C12A-C11A-C15A-F9'	22.9(19)
C12A-C13A-C16A-F12'	114.4(16)
C14A-C13A-C16A-F12'	-64.1(19)
C12A-C13A-C16A-F10A	-86.1(18)
C14A-C13A-C16A-F10A	95.4(17)
C12A-C13A-C16A-F10'	-26.5(19)
C14A-C13A-C16A-F10'	155.0(14)
C12A-C13A-C16A-F12A	144.0(13)
C14A-C13A-C16A-F12A	-34.5(17)
C12A-C13A-C16A-F11A	34.3(16)
C14A-C13A-C16A-F11A	-144.3(12)
C12A-C13A-C16A-F11'	-130.6(13)

C14A-C13A-C16A-F11'	50.9(15)
C25A-B1A-C17A-C18A	-158.1(10)
C9A-B1A-C17A-C18A	-38.5(13)
C1A-B1A-C17A-C18A	83.6(11)
C25"-B1A-C17A-C18A	-151.9(11)
C25A-B1A-C17A-C22A	22.1(13)
C9A-B1A-C17A-C22A	141.6(9)
C1A-B1A-C17A-C22A	-96.3(10)
C25"-B1A-C17A-C22A	28.2(14)
C22A-C17A-C18A-C19A	-1.1(16)
B1A-C17A-C18A-C19A	179.0(10)
C17A-C18A-C19A-C20A	0.1(19)
C17A-C18A-C19A-C23A	-179.0(11)
C18A-C19A-C20A-C21A	1.1(18)
C23A-C19A-C20A-C21A	-179.8(11)
C19A-C20A-C21A-C22A	-1.1(17)
C19A-C20A-C21A-C24A	-178.3(10)
C20A-C21A-C22A-C17A	0.0(17)
C24A-C21A-C22A-C17A	177.1(9)
C18A-C17A-C22A-C21A	1.1(15)
B1A-C17A-C22A-C21A	-179.0(9)
C20A-C19A-C23A-F15A	-125.0(16)
C18A-C19A-C23A-F15A	54.2(19)
C20A-C19A-C23A-F14'	93.7(18)
C18A-C19A-C23A-F14'	-87.2(18)
C20A-C19A-C23A-F14A	6.6(18)
C18A-C19A-C23A-F14A	-174.2(13)
C20A-C19A-C23A-F15'	-142.0(15)
C18A-C19A-C23A-F15'	37.1(19)
C20A-C19A-C23A-F13'	-31.8(17)
C18A-C19A-C23A-F13'	147.3(14)
C20A-C19A-C23A-F13A	116.4(13)
C18A-C19A-C23A-F13A	-64.5(15)
C22A-C21A-C24A-F16A	15.8(16)
C20A-C21A-C24A-F16A	-166.9(13)
C22A-C21A-C24A-F17A	-113.5(13)
C20A-C21A-C24A-F17A	63.7(15)
C22A-C21A-C24A-F18'	39.4(16)

C20A-C21A-C24A-F18'	-143.3(13)
C22A-C21A-C24A-F16'	-77.1(15)
C20A-C21A-C24A-F16'	100.2(14)
C22A-C21A-C24A-F17'	164.0(14)
C20A-C21A-C24A-F17'	-18.7(17)
C22A-C21A-C24A-F18A	134.9(11)
C20A-C21A-C24A-F18A	-47.9(14)
C17A-B1A-C25A-C30A	-146(5)
C9A-B1A-C25A-C30A	91(5)
C1A-B1A-C25A-C30A	-32(5)
C17A-B1A-C25A-C26A	59.3(18)
C9A-B1A-C25A-C26A	-63.6(18)
C1A-B1A-C25A-C26A	173.4(17)
C30A-C25A-C26A-C27A	18(6)
B1A-C25A-C26A-C27A	176(2)
C25A-C26A-C27A-C28A	-5(6)
C25A-C26A-C27A-C31A	165(2)
C26A-C27A-C28A-C29A	-10(9)
C31A-C27A-C28A-C29A	-179(4)
C27A-C28A-C29A-C30A	11(10)
C27A-C28A-C29A-C32A	-174(6)
C26A-C25A-C30A-C29A	-18(9)
B1A-C25A-C30A-C29A	-173(4)
C28A-C29A-C30A-C25A	4(11)
C32A-C29A-C30A-C25A	-172(7)
C28A-C27A-C31A-F19A	-20(5)
C26A-C27A-C31A-F19A	170(3)
C28A-C27A-C31A-F21A	111(5)
C26A-C27A-C31A-F21A	-59(3)
C28A-C27A-C31A-F20A	-137(5)
C26A-C27A-C31A-F20A	53(3)
C28A-C29A-C32A-F22A	94(5)
C30A-C29A-C32A-F22A	-91(6)
C28A-C29A-C32A-F24A	-130(5)
C30A-C29A-C32A-F24A	46(9)
C28A-C29A-C32A-F23A	-20(9)
C30A-C29A-C32A-F23A	156(6)
C17A-B1A-C25"-C30"	-124(6)

C9A-B1A-C25"-C30"	115(6)
C1A-B1A-C25"-C30"	-4(6)
C17A-B1A-C25"-C26"	31(2)
C9A-B1A-C25"-C26"	-91(2)
C1A-B1A-C25"-C26"	151(2)
C30"-C25"-C26"-C27"	-20(7)
B1A-C25"-C26"-C27"	-178(3)
C25"-C26"-C27"-C28"	7(8)
C25"-C26"-C27"-C31"	-162(3)
C26"-C27"-C28"-C29"	9(11)
C31"-C27"-C28"-C29"	178(5)
C27"-C28"-C29"-C30"	-11(11)
C27"-C28"-C29"-C32"	174(7)
C26"-C25"-C30"-C29"	18(11)
B1A-C25"-C30"-C29"	174(5)
C28"-C29"-C30"-C25"	-3(12)
C32"-C29"-C30"-C25"	172(7)
C28"-C27"-C31"-F19"	39(6)
C26"-C27"-C31"-F19"	-151(3)
C28"-C27"-C31"-F21"	170(6)
C26"-C27"-C31"-F21"	-20(4)
C28"-C27"-C31"-F20"	-77(6)
C26"-C27"-C31"-F20"	93(3)
C28"-C29"-C32"-F22"	-90(6)
C30"-C29"-C32"-F22"	94(6)
C28"-C29"-C32"-F24"	45(9)
C30"-C29"-C32"-F24"	-130(6)
C28"-C29"-C32"-F23"	155(6)
C30"-C29"-C32"-F23"	-20(10)

[(2′,4′,6′-Triisopropyl-1,1′-biphenyl-2-yl)di-*tert*-butylphosphine](3,5-bis(trifluoromethyl)phenyl)gold (21) CCDC: 1572064.

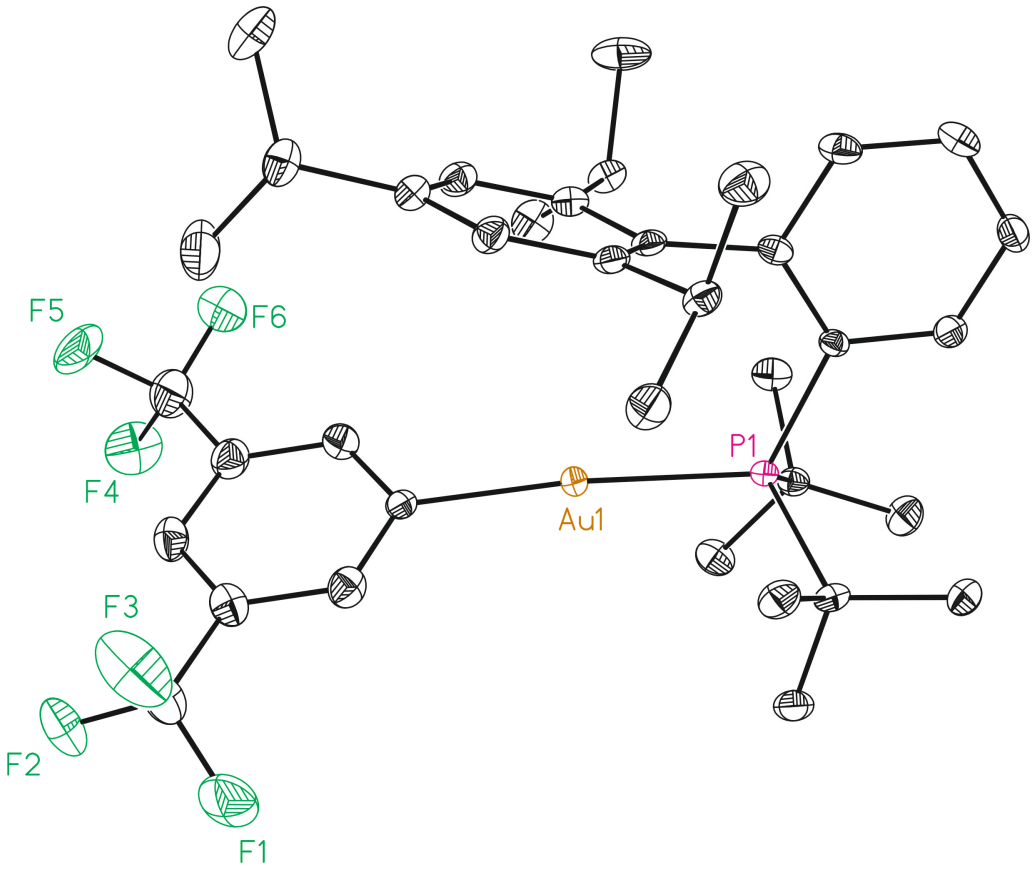


Table 1. Crystal data and structure refinement for SFC-A-51.

Identification code	SFC-A-51	
Empirical formula	C9.55 H12.39 Au0.26 F1.55 P0.26	
Formula weight	215.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 17.1985(4)Å	a= 90°.
	b = 12.3112(3)Å	b = 91.514(2)°.
	c = 33.5442(11)Å	g = 90°.
Volume	7100.0(3) $Å^3$	
Z	31	
Density (calculated)	1.562 Mg/m^3	
Absorption coefficient	4.245 mm^{-1}	
F(000)	3344	
Crystal size	0.30 x 0.15 x 0.08 mm^3	
Theta range for data collection	2.354 to 32.384°.	

Index ranges	-25<=h<=24,-15<=k<=18,-48<=l<=49
Reflections collected	37560
Independent reflections	11836[R(int) = 0.0353]
Completeness to theta =32.384°	93.0%
Absorption correction	Empirical
Max. and min. transmission	0.728 and 0.56
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11836/ 246/ 472
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0668
R indices (all data)	R1 = 0.0451, wR2 = 0.0704
Largest diff. peak and hole	1.989 and -0.905 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for SFC-A-51.

Bond lengths----	
Au1-C1	2.088(3)
Au1-P1	2.2966(7)
P1-C9	1.845(3)
P1-C34	1.890(3)
P1-C30	1.899(3)
C1-C2	1.349(4)
C1-C6	1.411(4)
C2-C3	1.400(4)
C2-H2	0.9300
C3-C4	1.384(4)
C3-C7	1.499(4)
C4-C5	1.392(4)
C4-H4	0.9300
C5-C6	1.383(4)
C5-C8	1.494(5)
C6-H6	0.9300
C7-F2	1.334(4)
C7-F3	1.341(4)
C7-F1	1.366(4)
C8-F4	1.311(6)
C8-F5"	1.313(8)
C8-F5'	1.331(8)
C8-F4"	1.338(8)

C8-F6'	1.348(8)
C8-F6	1.359(5)
C8-F4'	1.361(7)
C8-F6"	1.383(8)
C8-F5	1.397(5)
C9-C10	1.401(4)
C9-C14	1.416(4)
C10-C11	1.387(4)
C10-H10	0.9300
C11-C12	1.382(4)
C11-H11	0.9300
C12-C13	1.387(4)
C12-H12	0.9300
C13-C14	1.402(4)
C13-H13	0.9300
C14-C15	1.505(4)
C15-C16	1.416(4)
C15-C20	1.418(4)
C16-C17	1.388(4)
C16-C21	1.521(4)
C17-C18	1.388(4)
C17-H17	0.9300
C18-C19	1.394(4)
C18-C24	1.523(4)
C19-C20	1.389(4)
C19-H19	0.9300
C20-C27	1.522(4)
C21-C23	1.530(4)
C21-C22	1.537(4)
C21-H21	0.9800
C22-H22A	0.9600
C22-H22B	0.9600
C22-H22C	0.9600
C23-H23A	0.9600
C23-H23B	0.9600
C23-H23C	0.9600
C24-C26	1.519(5)
C24-C25	1.532(5)

C24-H24	0.9800
C25-H25A	0.9600
C25-H25B	0.9600
C25-H25C	0.9600
C26-H26A	0.9600
C26-H26B	0.9600
C26-H26C	0.9600
C27-C29	1.524(4)
C27-C28	1.535(4)
C27-H27	0.9800
C28-H28A	0.9600
C28-H28B	0.9600
C28-H28C	0.9600
C29-H29A	0.9600
C29-H29B	0.9600
C29-H29C	0.9600
C30-C32	1.531(4)
C30-C31	1.531(4)
C30-C33	1.542(4)
C31-H31A	0.9600
C31-H31B	0.9600
C31-H31C	0.9600
C32-H32A	0.9600
C32-H32B	0.9600
C32-H32C	0.9600
C33-H33A	0.9600
C33-H33B	0.9600
C33-H33C	0.9600
C34-C35	1.528(4)
C34-C36	1.541(4)
C34-C37	1.542(4)
C35-H35A	0.9600
C35-H35B	0.9600
C35-H35C	0.9600
C36-H36A	0.9600
C36-H36B	0.9600
C36-H36C	0.9600
C37-H37A	0.9600

C37-H37B	0.9600
C37-H37C	0.9600

Angles----------

C1-Au1-P1	174.45(7)
C9-P1-C34	107.14(12)
C9-P1-C30	106.20(11)
C34-P1-C30	110.94(12)
C9-P1-Au1	115.32(9)
C34-P1-Au1	107.78(9)
C30-P1-Au1	109.46(9)
C2-C1-C6	118.6(3)
C2-C1-Au1	123.4(2)
C6-C1-Au1	117.6(2)
C1-C2-C3	121.6(3)
C1-C2-H2	119.2
C3-C2-H2	119.2
C4-C3-C2	120.5(3)
C4-C3-C7	119.4(3)
C2-C3-C7	120.1(3)
C3-C4-C5	118.0(3)
C3-C4-H4	121.0
C5-C4-H4	121.0
C6-C5-C4	121.2(3)
C6-C5-C8	120.3(3)
C4-C5-C8	118.4(3)
C5-C6-C1	120.0(3)
C5-C6-H6	120.0
C1-C6-H6	120.0
F2-C7-F3	105.6(3)
F2-C7-F1	107.1(3)
F3-C7-F1	106.4(3)
F2-C7-C3	112.7(3)
F3-C7-C3	112.7(3)
F1-C7-C3	111.9(3)
F5"-C8-F4"	109.3(8)
F5'-C8-F6'	106.0(7)
F4-C8-F6	109.5(4)

F5'-C8-F4'	105.3(6)
F6'-C8-F4'	106.3(7)
F5"-C8-F6"	106.1(7)
F4"-C8-F6"	102.9(7)
F4-C8-F5	103.2(4)
F6-C8-F5	103.2(4)
F4-C8-C5	114.3(4)
F5"-C8-C5	116.8(8)
F5'-C8-C5	117.7(7)
F4"-C8-C5	112.9(8)
F6'-C8-C5	108.1(8)
F6-C8-C5	116.8(4)
F4'-C8-C5	112.8(6)
F6"-C8-C5	107.7(6)
F5-C8-C5	108.3(4)
C10-C9-C14	118.5(2)
C10-C9-P1	117.98(19)
C14-C9-P1	123.48(19)
C11-C10-C9	122.4(3)
C11-C10-H10	118.8
C9-C10-H10	118.8
C12-C11-C10	119.3(3)
C12-C11-H11	120.3
C10-C11-H11	120.3
C11-C12-C13	119.0(3)
C11-C12-H12	120.5
C13-C12-H12	120.5
C12-C13-C14	123.0(3)
C12-C13-H13	118.5
C14-C13-H13	118.5
C13-C14-C9	117.6(2)
C13-C14-C15	114.0(2)
C9-C14-C15	128.4(2)
C16-C15-C20	119.1(2)
C16-C15-C14	119.1(2)
C20-C15-C14	120.9(2)
C17-C16-C15	119.2(3)
C17-C16-C21	118.9(2)

C15-C16-C21	121.8(2)
C18-C17-C16	122.7(3)
C18-C17-H17	118.7
C16-C17-H17	118.7
C17-C18-C19	117.3(3)
C17-C18-C24	120.5(3)
C19-C18-C24	122.2(3)
C20-C19-C18	122.8(3)
C20-C19-H19	118.6
C18-C19-H19	118.6
C19-C20-C15	118.9(3)
C19-C20-C27	119.7(3)
C15-C20-C27	121.3(2)
C16-C21-C23	111.3(2)
C16-C21-C22	112.1(2)
C23-C21-C22	109.4(2)
C16-C21-H21	108.0
C23-C21-H21	108.0
C22-C21-H21	108.0
C21-C22-H22A	109.5
C21-C22-H22B	109.5
H22A-C22-H22B	109.5
C21-C22-H22C	109.5
H22A-C22-H22C	109.5
H22B-C22-H22C	109.5
C21-C23-H23A	109.5
C21-C23-H23B	109.5
H23A-C23-H23B	109.5
C21-C23-H23C	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C26-C24-C18	111.7(3)
C26-C24-C25	111.5(3)
C18-C24-C25	111.6(3)
C26-C24-H24	107.2
C18-C24-H24	107.2
C25-C24-H24	107.2
C24-C25-H25A	109.5

C24-C25-H25B	109.5
H25A-C25-H25B	109.5
C24-C25-H25C	109.5
H25A-C25-H25C	109.5
H25B-C25-H25C	109.5
C24-C26-H26A	109.5
C24-C26-H26B	109.5
H26A-C26-H26B	109.5
C24-C26-H26C	109.5
H26A-C26-H26C	109.5
H26B-C26-H26C	109.5
C20-C27-C29	113.0(2)
C20-C27-C28	110.7(2)
C29-C27-C28	110.2(3)
C20-C27-H27	107.5
C29-C27-H27	107.5
C28-C27-H27	107.5
C27-C28-H28A	109.5
C27-C28-H28B	109.5
H28A-C28-H28B	109.5
C27-C28-H28C	109.5
H28A-C28-H28C	109.5
H28B-C28-H28C	109.5
C27-C29-H29A	109.5
C27-C29-H29B	109.5
H29A-C29-H29B	109.5
C27-C29-H29C	109.5
H29A-C29-H29C	109.5
H29B-C29-H29C	109.5
C32-C30-C31	108.7(2)
C32-C30-C33	108.5(2)
C31-C30-C33	107.4(2)
C32-C30-P1	116.4(2)
C31-C30-P1	107.38(18)
C33-C30-P1	108.13(18)
C30-C31-H31A	109.5
C30-C31-H31B	109.5
H31A-C31-H31B	109.5

C30-C31-H31C	109.5
H31A-C31-H31C	109.5
H31B-C31-H31C	109.5
C30-C32-H32A	109.5
C30-C32-H32B	109.5
H32A-C32-H32B	109.5
C30-C32-H32C	109.5
H32A-C32-H32C	109.5
H32B-C32-H32C	109.5
C30-C33-H33A	109.5
C30-C33-H33B	109.5
H33A-C33-H33B	109.5
C30-C33-H33C	109.5
H33A-C33-H33C	109.5
H33B-C33-H33C	109.5
C35-C34-C36	109.5(2)
C35-C34-C37	108.6(2)
C36-C34-C37	107.8(2)
C35-C34-P1	116.57(19)
C36-C34-P1	108.8(2)
C37-C34-P1	105.24(18)
C34-C35-H35A	109.5
C34-C35-H35B	109.5
H35A-C35-H35B	109.5
C34-C35-H35C	109.5
H35A-C35-H35C	109.5
H35B-C35-H35C	109.5
C34-C36-H36A	109.5
C34-C36-H36B	109.5
H36A-C36-H36B	109.5
C34-C36-H36C	109.5
H36A-C36-H36C	109.5
H36B-C36-H36C	109.5
C34-C37-H37A	109.5
C34-C37-H37B	109.5
H37A-C37-H37B	109.5
C34-C37-H37C	109.5
H37A-C37-H37C	109.5

H37B-C37-H37C 109.5

Table 3. Torsion angles [°] for SFC-A-51.

C6-C1-C2-C3	-3.1(4)
Au1-C1-C2-C3	-175.6(2)
C1-C2-C3-C4	2.4(5)
C1-C2-C3-C7	-176.9(3)
C2-C3-C4-C5	-0.8(5)
C7-C3-C4-C5	178.5(3)
C3-C4-C5-C6	0.1(5)
C3-C4-C5-C8	-179.0(3)
C4-C5-C6-C1	-0.9(5)
C8-C5-C6-C1	178.3(3)
C2-C1-C6-C5	2.4(4)
Au1-C1-C6-C5	175.3(2)
C4-C3-C7-F2	18.8(4)
C2-C3-C7-F2	-161.8(3)
C4-C3-C7-F3	-100.6(4)
C2-C3-C7-F3	78.8(4)
C4-C3-C7-F1	139.6(3)
C2-C3-C7-F1	-41.1(4)
C6-C5-C8-F4	117.7(5)
C4-C5-C8-F4	-63.2(5)
C6-C5-C8-F5"	-164.4(10)
C4-C5-C8-F5"	14.7(10)
C6-C5-C8-F5'	-99.8(8)
C4-C5-C8-F5'	79.4(8)
C6-C5-C8-F4"	-36.4(8)
C4-C5-C8-F4"	142.8(7)
C6-C5-C8-F6'	140.3(7)
C4-C5-C8-F6'	-40.5(7)
C6-C5-C8-F6	-12.0(5)
C4-C5-C8-F6	167.1(4)
C6-C5-C8-F4'	23.2(8)
C4-C5-C8-F4'	-157.7(7)
C6-C5-C8-F6"	76.5(8)
C4-C5-C8-F6"	-104.4(8)

C6-C5-C8-F5	-127.9(4)
C4-C5-C8-F5	51.3(5)
C34-P1-C9-C10	62.6(2)
C30-P1-C9-C10	-56.0(2)
Au1-P1-C9-C10	-177.45(17)
C34-P1-C9-C14	-118.7(2)
C30-P1-C9-C14	122.7(2)
Au1-P1-C9-C14	1.3(2)
C14-C9-C10-C11	0.2(4)
P1-C9-C10-C11	179.0(2)
C9-C10-C11-C12	-0.4(4)
C10-C11-C12-C13	0.1(4)
C11-C12-C13-C14	0.3(4)
C12-C13-C14-C9	-0.4(4)
C12-C13-C14-C15	177.5(3)
C10-C9-C14-C13	0.2(4)
P1-C9-C14-C13	-178.5(2)
C10-C9-C14-C15	-177.4(3)
P1-C9-C14-C15	3.9(4)
C13-C14-C15-C16	-79.0(3)
C9-C14-C15-C16	98.6(3)
C13-C14-C15-C20	89.7(3)
C9-C14-C15-C20	-92.6(3)
C20-C15-C16-C17	1.4(4)
C14-C15-C16-C17	170.4(2)
C20-C15-C16-C21	-174.7(2)
C14-C15-C16-C21	-5.8(4)
C15-C16-C17-C18	-1.2(4)
C21-C16-C17-C18	175.0(3)
C16-C17-C18-C19	0.9(4)
C16-C17-C18-C24	-177.9(3)
C17-C18-C19-C20	-0.9(4)
C24-C18-C19-C20	177.9(3)
C18-C19-C20-C15	1.1(4)
C18-C19-C20-C27	-175.2(3)
C16-C15-C20-C19	-1.4(4)
C14-C15-C20-C19	-170.1(2)
C16-C15-C20-C27	174.8(2)

C14-C15-C20-C27	6.1(4)
C17-C16-C21-C23	-74.7(3)
C15-C16-C21-C23	101.4(3)
C17-C16-C21-C22	48.1(3)
C15-C16-C21-C22	-135.7(3)
C17-C18-C24-C26	-111.7(3)
C19-C18-C24-C26	69.6(4)
C17-C18-C24-C25	122.8(3)
C19-C18-C24-C25	-56.0(4)
C19-C20-C27-C29	-49.6(4)
C15-C20-C27-C29	134.1(3)
C19-C20-C27-C28	74.6(4)
C15-C20-C27-C28	-101.7(3)
C9-P1-C30-C32	75.5(2)
C34-P1-C30-C32	-40.6(2)
Au1-P1-C30-C32	-159.39(18)
C9-P1-C30-C31	-46.6(2)
C34-P1-C30-C31	-162.67(19)
Au1-P1-C30-C31	78.52(19)
C9-P1-C30-C33	-162.14(19)
C34-P1-C30-C33	81.8(2)
Au1-P1-C30-C33	-37.0(2)
C9-P1-C34-C35	-44.1(2)
C30-P1-C34-C35	71.4(2)
Au1-P1-C34-C35	-168.79(19)
C9-P1-C34-C36	-168.38(19)
C30-P1-C34-C36	-52.9(2)
Au1-P1-C34-C36	66.9(2)
C9-P1-C34-C37	76.3(2)
C30-P1-C34-C37	-168.20(18)
Au1-P1-C34-C37	-48.39(19)

Bis(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (20) CCDC: 1572068.

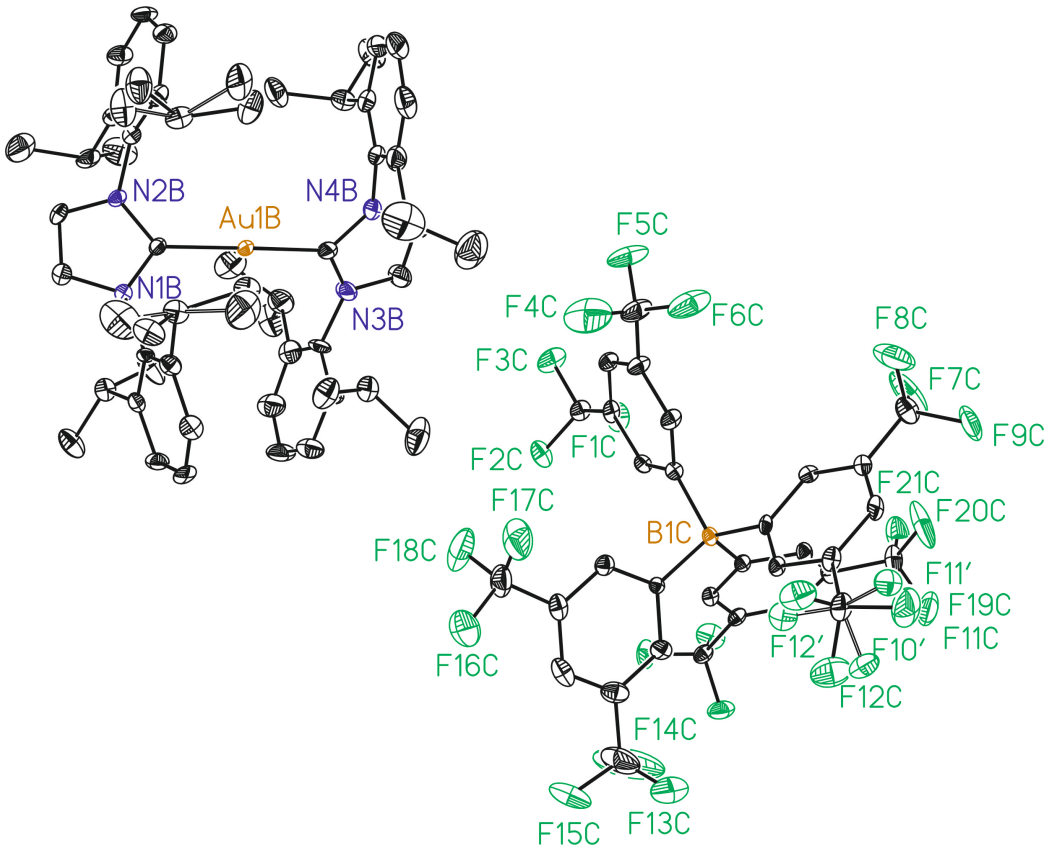


Table 1. Crystal data and structure refinement for SFC-A-94.

Identification code	SFC-A-94	
Empirical formula	C172 H168 Au2 B2 F48 N8	
Formula weight	3674.69	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 24.1971(5)Å	a= 90°.
	b = 28.4333(5)Å	b = 94.219(2)°.
	c = 24.4659(5)Å	g = 90°.
Volume	16787.0(6) $Å^3$	
Z	4	
Density (calculated)	1.454 Mg/m^3	
Absorption coefficient	1.852 mm^{-1}	
F(000)	7424	
Crystal size	0.15 x 0.06 x 0.03	mm^3
Theta range for data collection	2.285 to 32.356°.	
Index ranges	-35<=h<=22,-41<=k<=25,-36<=l<=36	

Reflections collected	156543
Independent reflections	54217[R(int) = 0.0614]
Completeness to theta =32.356°	90.3%
Absorption correction	Empirical
Max. and min. transmission	0.947 and 0.728
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	54217/ 1172/ 2335
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0762, wR2 = 0.1310
R indices (all data)	R1 = 0.1436, wR2 = 0.1487
Largest diff. peak and hole	2.781 and -3.183 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for SFC-A-94.

Bond lengths----

Au1A-C28A	2.032(5)
Au1A-C1A	2.034(5)
N1A-C1A	1.359(7)
N1A-C2A	1.388(7)
N1A-C4A	1.450(7)
N2A-C1A	1.345(7)
N2A-C3A	1.393(7)
N2A-C16A	1.449(7)
N3A-C28A	1.363(7)
N3A-C29A	1.379(7)
N3A-C31A	1.436(7)
N4A-C28A	1.357(7)
N4A-C30A	1.380(7)
N4A-C43A	1.452(7)
C2A-C3A	1.345(8)
C4A-C9A	1.385(8)
C4A-C5A	1.399(8)
C5A-C6A	1.377(8)
C5A-C10A	1.522(7)
C6A-C7A	1.383(9)
C7A-C8A	1.380(9)
C8A-C9A	1.390(9)
C9A-C13A	1.529(9)
C10A-C12A	1.522(8)

C10A-C11A	1.542(9)
C13A-C14A	1.517(9)
C13A-C15A	1.522(9)
C16A-C17A	1.391(8)
C16A-C21A	1.392(8)
C17A-C18A	1.394(8)
C17A-C22A	1.527(8)
C18A-C19A	1.372(8)
C19A-C20A	1.380(8)
C20A-C21A	1.400(8)
C21A-C25A	1.522(8)
C22A-C24A	1.530(8)
C22A-C23A	1.535(8)
C25A-C26A	1.516(10)
C25A-C27A	1.522(10)
C29A-C30A	1.350(8)
C31A-C32A	1.395(9)
C31A-C36A	1.397(9)
C32A-C33A	1.403(9)
C32A-C37A	1.521(9)
C33A-C34A	1.381(10)
C34A-C35A	1.370(10)
C35A-C36A	1.386(9)
C36A-C40A	1.521(9)
C37A-C38A	1.510(9)
C37A-C39'	1.521(9)
C37A-C39A	1.524(9)
C37A-C38'	1.532(9)
C40A-C41A	1.525(9)
C40A-C42A	1.530(9)
C43A-C48A	1.394(9)
C43A-C44A	1.406(9)
C44A-C45A	1.397(9)
C44A-C49A	1.522(9)
C45A-C46A	1.377(9)
C46A-C47A	1.367(9)
C47A-C48A	1.405(8)
C48A-C52A	1.521(9)

C49A-C51A	1.513(10)
C49A-C50A	1.536(10)
C52A-C54A	1.525(9)
C52A-C53A	1.537(9)
Au1B-C28B	2.024(6)
Au1B-C1B	2.037(5)
N1B-C1B	1.341(7)
N1B-C2B	1.383(7)
N1B-C4B	1.454(7)
N2B-C1B	1.357(7)
N2B-C3B	1.366(7)
N2B-C16B	1.455(7)
N3B-C28B	1.361(8)
N3B-C29B	1.385(8)
N3B-C31B	1.436(7)
N4B-C28B	1.361(8)
N4B-C30B	1.398(9)
N4B-C43B	1.446(8)
C2B-C3B	1.347(8)
C4B-C9B	1.395(8)
C4B-C5B	1.403(8)
C5B-C6B	1.396(8)
C5B-C10B	1.518(8)
C6B-C7B	1.380(8)
C7B-C8B	1.384(8)
C8B-C9B	1.406(8)
C9B-C13B	1.517(8)
C10B-C11B	1.521(8)
C10B-C12B	1.528(8)
C13B-C14"	1.521(9)
C13B-C15B	1.527(7)
C13B-C14B	1.530(7)
C13B-C15"	1.530(9)
C16B-C21B	1.381(8)
C16B-C17B	1.395(8)
C17B-C18B	1.384(8)
C17B-C22B	1.536(8)
C18B-C19B	1.399(8)

C19B-C20B	1.371(8)
C20B-C21B	1.389(8)
C21B-C25B	1.531(8)
C22B-C23B	1.509(8)
C22B-C24"	1.512(9)
C22B-C24B	1.523(8)
C22B-C23"	1.524(9)
C25B-C27B	1.520(10)
C25B-C26B	1.544(9)
C29B-C30B	1.346(10)
C31B-C36B	1.400(10)
C31B-C32B	1.419(10)
C32B-C33B	1.371(10)
C32B-C37B	1.527(10)
C33B-C34B	1.363(10)
C34B-C35B	1.377(10)
C35B-C36B	1.400(9)
C36B-C40B	1.513(10)
C37B-C38B	1.521(10)
C37B-C39B	1.546(10)
C40B-C41B	1.521(10)
C40B-C42B	1.525(9)
C43B-C48B	1.400(9)
C43B-C44B	1.401(10)
C44B-C45B	1.378(10)
C44B-C49B	1.519(10)
C45B-C46B	1.394(11)
C46B-C47B	1.372(10)
C47B-C48B	1.408(9)
C48B-C52B	1.502(9)
C49B-C51B	1.470(11)
C49B-C50B	1.558(11)
C52B-C54B	1.526(10)
C52B-C53B	1.528(9)
B1C-C25C	1.641(8)
B1C-C1C	1.642(8)
B1C-C9C	1.644(7)
B1C-C17C	1.646(8)

C1C-C2C	1.395(7)
C1C-C6C	1.406(7)
C2C-C3C	1.393(7)
C3C-C4C	1.379(8)
C3C-C7C	1.507(7)
C4C-C5C	1.384(7)
C5C-C6C	1.387(8)
C5C-C8C	1.501(8)
C7C-F1C	1.333(6)
C7C-F2C	1.336(6)
C7C-F3C	1.341(6)
C8C-F6C	1.325(8)
C8C-F4C	1.329(9)
C8C-F5C	1.329(7)
C9C-C14C	1.390(7)
C9C-C10C	1.401(7)
C10C-C11C	1.396(7)
C11C-C12C	1.393(7)
C11C-C15C	1.482(8)
C12C-C13C	1.376(8)
C13C-C14C	1.403(7)
C13C-C16C	1.490(7)
C15C-F7C	1.308(7)
C15C-F8C	1.326(7)
C15C-F9C	1.339(7)
C16C-F10'	1.313(7)
C16C-F10C	1.316(6)
C16C-F12'	1.332(7)
C16C-F11C	1.336(6)
C16C-F11'	1.357(7)
C16C-F12C	1.363(7)
C17C-C18C	1.386(7)
C17C-C22C	1.394(7)
C18C-C19C	1.393(8)
C19C-C20C	1.377(9)
C19C-C23C	1.500(10)
C20C-C21C	1.387(9)
C21C-C22C	1.383(8)

C21C-C24C	1.503(9)
C23C-F14C	1.315(11)
C23C-F15C	1.317(9)
C23C-F13C	1.324(10)
C24C-F18C	1.317(8)
C24C-F17C	1.334(8)
C24C-F16C	1.337(8)
C25C-C30C	1.402(7)
C25C-C26C	1.406(7)
C26C-C27C	1.387(7)
C27C-C28C	1.394(7)
C27C-C31C	1.499(8)
C28C-C29C	1.378(8)
C29C-C30C	1.385(7)
C29C-C32C	1.505(7)
C31C-F20C	1.323(7)
C31C-F21C	1.331(7)
C31C-F19C	1.335(8)
C32C-F24C	1.331(7)
C32C-F23C	1.337(6)
C32C-F22C	1.345(6)
B1D-C25D	1.614(9)
B1D-C17D	1.617(10)
B1D-C9D	1.646(8)
B1D-C1D	1.749(7)
B1D-C1D'	1.779(9)
C1D-C6D	1.370(9)
C1D-C2D	1.410(10)
C2D-C3D	1.384(10)
C3D-C4D	1.385(10)
C3D-C7D	1.480(12)
C4D-C5D	1.391(10)
C5D-C6D	1.386(9)
C5D-C8D	1.494(8)
C7D-F1D	1.251(14)
C7D-F2D	1.265(13)
C7D-F3D	1.307(13)
C8D-F6D	1.331(9)

C8D-F4D	1.335(10)
C8D-F5D	1.372(10)
C1D'-C6D'	1.372(10)
C1D'-C2D'	1.413(11)
C2D'-C3D'	1.386(10)
C3D'-C4D'	1.386(10)
C3D'-C7D'	1.481(12)
C4D'-C5D'	1.392(10)
C5D'-C6D'	1.389(9)
C5D'-C8D'	1.493(9)
C7D'-F1D'	1.253(15)
C7D'-F2D'	1.262(13)
C7D'-F3D'	1.312(14)
C8D'-F6D'	1.331(10)
C8D'-F4D'	1.337(11)
C8D'-F5D'	1.373(11)
C9D-C10D	1.392(9)
C9D-C14D	1.405(8)
C10D-C11D	1.388(8)
C11D-C12D	1.382(9)
C11D-C15D	1.483(9)
C12D-C13D	1.387(9)
C13D-C14D	1.398(8)
C13D-C16D	1.485(9)
C15D-F9D	1.341(8)
C15D-F8D	1.344(7)
C15D-F7D	1.351(8)
C16D-F10D	1.310(9)
C16D-F12D	1.313(8)
C16D-F11D	1.375(8)
C17D-C18D	1.404(9)
C17D-C22D	1.407(9)
C18D-C19D	1.400(9)
C19D-C20D	1.377(9)
C19D-C23D	1.530(11)
C20D-C21D	1.369(10)
C21D-C22D	1.376(10)
C21D-C24D	1.505(10)

C23D-F13D	1.294(10)
C23D-F14D	1.311(9)
C23D-F15D	1.358(11)
C24D-F18D	1.315(10)
C24D-F17D	1.317(10)
C24D-F16D	1.330(9)
C25D-C30D	1.393(9)
C25D-C26D	1.402(8)
C26D-C27D	1.389(8)
C27D-C28D	1.386(8)
C27D-C31D	1.500(8)
C28D-C29D	1.398(8)
C29D-C30D	1.380(9)
C29D-C32D	1.476(9)
C31D-F20D	1.312(7)
C31D-F19D	1.318(7)
C31D-F21D	1.326(7)
C32D-F22D	1.282(10)
C32D-F24D	1.320(8)
C32D-F23D	1.326(9)

Angles----------

C28A-Au1A-C1A	178.5(2)
C1A-N1A-C2A	111.0(5)
C1A-N1A-C4A	126.7(5)
C2A-N1A-C4A	122.3(5)
C1A-N2A-C3A	110.8(5)
C1A-N2A-C16A	128.5(5)
C3A-N2A-C16A	120.7(5)
C28A-N3A-C29A	111.8(5)
C28A-N3A-C31A	126.4(5)
C29A-N3A-C31A	121.3(5)
C28A-N4A-C30A	111.4(5)
C28A-N4A-C43A	127.1(5)
C30A-N4A-C43A	121.5(5)
N2A-C1A-N1A	104.8(5)
N2A-C1A-Au1A	127.5(4)
N1A-C1A-Au1A	127.6(4)

C3A-C2A-N1A	106.3(5)
C2A-C3A-N2A	107.0(5)
C9A-C4A-C5A	123.4(5)
C9A-C4A-N1A	118.5(5)
C5A-C4A-N1A	117.9(5)
C6A-C5A-C4A	117.2(5)
C6A-C5A-C10A	120.5(5)
C4A-C5A-C10A	122.1(5)
C5A-C6A-C7A	121.2(5)
C8A-C7A-C6A	120.0(6)
C7A-C8A-C9A	121.2(6)
C4A-C9A-C8A	117.0(5)
C4A-C9A-C13A	121.0(6)
C8A-C9A-C13A	121.9(6)
C12A-C10A-C5A	110.6(5)
C12A-C10A-C11A	107.7(6)
C5A-C10A-C11A	113.1(5)
C14A-C13A-C15A	112.7(6)
C14A-C13A-C9A	109.7(6)
C15A-C13A-C9A	113.1(6)
C17A-C16A-C21A	123.3(5)
C17A-C16A-N2A	117.7(5)
C21A-C16A-N2A	118.7(5)
C16A-C17A-C18A	117.6(5)
C16A-C17A-C22A	121.6(5)
C18A-C17A-C22A	120.8(5)
C19A-C18A-C17A	120.5(5)
C18A-C19A-C20A	121.1(6)
C19A-C20A-C21A	120.7(6)
C16A-C21A-C20A	116.9(5)
C16A-C21A-C25A	123.0(5)
C20A-C21A-C25A	120.1(6)
C17A-C22A-C24A	113.1(5)
C17A-C22A-C23A	110.1(5)
C24A-C22A-C23A	109.5(5)
C26A-C25A-C21A	109.8(5)
C26A-C25A-C27A	109.6(7)
C21A-C25A-C27A	112.3(5)

N4A-C28A-N3A	103.6(4)
N4A-C28A-Au1A	128.1(4)
N3A-C28A-Au1A	128.3(4)
C30A-C29A-N3A	106.2(5)
C29A-C30A-N4A	107.0(5)
C32A-C31A-C36A	123.1(6)
C32A-C31A-N3A	117.7(5)
C36A-C31A-N3A	118.8(5)
C31A-C32A-C33A	117.3(6)
C31A-C32A-C37A	123.4(6)
C33A-C32A-C37A	119.3(6)
C34A-C33A-C32A	120.4(6)
C35A-C34A-C33A	120.6(6)
C34A-C35A-C36A	121.8(7)
C35A-C36A-C31A	116.8(6)
C35A-C36A-C40A	120.9(6)
C31A-C36A-C40A	122.2(6)
C38A-C37A-C32A	116.3(9)
C32A-C37A-C39'	113.9(15)
C38A-C37A-C39A	111.5(9)
C32A-C37A-C39A	114.3(14)
C32A-C37A-C38'	104.9(8)
C39'-C37A-C38'	109.9(8)
C36A-C40A-C41A	112.3(6)
C36A-C40A-C42A	110.7(6)
C41A-C40A-C42A	110.9(6)
C48A-C43A-C44A	124.4(5)
C48A-C43A-N4A	117.7(5)
C44A-C43A-N4A	117.6(5)
C45A-C44A-C43A	116.0(6)
C45A-C44A-C49A	122.1(6)
C43A-C44A-C49A	122.0(6)
C46A-C45A-C44A	121.3(6)
C47A-C46A-C45A	120.9(6)
C46A-C47A-C48A	121.4(6)
C43A-C48A-C47A	116.0(6)
C43A-C48A-C52A	121.7(5)
C47A-C48A-C52A	122.3(6)

C51A-C49A-C44A	113.6(6)
C51A-C49A-C50A	110.8(6)
C44A-C49A-C50A	110.8(6)
C48A-C52A-C54A	110.2(6)
C48A-C52A-C53A	113.9(5)
C54A-C52A-C53A	110.1(5)
C28B-Au1B-C1B	175.4(2)
C1B-N1B-C2B	111.2(4)
C1B-N1B-C4B	127.2(4)
C2B-N1B-C4B	121.3(4)
C1B-N2B-C3B	110.6(4)
C1B-N2B-C16B	127.5(5)
C3B-N2B-C16B	121.4(4)
C28B-N3B-C29B	112.1(5)
C28B-N3B-C31B	126.5(5)
C29B-N3B-C31B	120.9(5)
C28B-N4B-C30B	110.9(5)
C28B-N4B-C43B	127.2(5)
C30B-N4B-C43B	121.9(5)
N1B-C1B-N2B	104.8(4)
N1B-C1B-Au1B	128.9(4)
N2B-C1B-Au1B	126.1(4)
C3B-C2B-N1B	106.0(5)
C2B-C3B-N2B	107.4(5)
C9B-C4B-C5B	123.6(5)
C9B-C4B-N1B	117.8(5)
C5B-C4B-N1B	118.3(5)
C6B-C5B-C4B	116.2(5)
C6B-C5B-C10B	122.5(5)
C4B-C5B-C10B	121.2(5)
C7B-C6B-C5B	121.9(5)
C6B-C7B-C8B	120.3(5)
C7B-C8B-C9B	120.6(5)
C4B-C9B-C8B	117.2(5)
C4B-C9B-C13B	123.2(5)
C8B-C9B-C13B	119.7(5)
C5B-C10B-C11B	110.7(5)
C5B-C10B-C12B	113.9(5)

C11B-C10B-C12B	109.6(5)
C9B-C13B-C14"	113.5(10)
C9B-C13B-C15B	112.2(6)
C9B-C13B-C14B	111.1(6)
C15B-C13B-C14B	110.0(6)
C9B-C13B-C15"	108.5(10)
C14"-C13B-C15"	109.8(8)
C21B-C16B-C17B	123.5(6)
C21B-C16B-N2B	118.4(5)
C17B-C16B-N2B	117.8(5)
C18B-C17B-C16B	117.6(5)
C18B-C17B-C22B	119.6(5)
C16B-C17B-C22B	122.8(5)
C17B-C18B-C19B	120.2(5)
C20B-C19B-C18B	120.0(6)
C19B-C20B-C21B	121.7(6)
C16B-C21B-C20B	116.9(5)
C16B-C21B-C25B	123.4(5)
C20B-C21B-C25B	119.7(5)
C23B-C22B-C24B	111.2(7)
C24"-C22B-C23"	110.7(7)
C23B-C22B-C17B	110.9(8)
C24"-C22B-C17B	109.1(9)
C24B-C22B-C17B	112.3(9)
C23"-C22B-C17B	111.2(9)
C27B-C25B-C21B	111.6(5)
C27B-C25B-C26B	109.9(6)
C21B-C25B-C26B	111.0(5)
N3B-C28B-N4B	103.8(5)
N3B-C28B-Au1B	127.0(4)
N4B-C28B-Au1B	129.0(4)
C30B-C29B-N3B	106.2(6)
C29B-C30B-N4B	107.0(6)
C36B-C31B-C32B	123.2(6)
C36B-C31B-N3B	117.3(6)
C32B-C31B-N3B	119.1(6)
C33B-C32B-C31B	116.6(7)
C33B-C32B-C37B	121.7(7)

C31B-C32B-C37B	121.8(6)
C34B-C33B-C32B	121.8(8)
C33B-C34B-C35B	121.3(7)
C34B-C35B-C36B	120.6(7)
C35B-C36B-C31B	116.5(7)
C35B-C36B-C40B	120.4(7)
C31B-C36B-C40B	123.1(6)
C38B-C37B-C32B	112.3(6)
C38B-C37B-C39B	107.7(6)
C32B-C37B-C39B	112.6(6)
C36B-C40B-C41B	112.3(6)
C36B-C40B-C42B	110.9(6)
C41B-C40B-C42B	109.8(6)
C48B-C43B-C44B	123.6(6)
C48B-C43B-N4B	116.5(6)
C44B-C43B-N4B	119.7(6)
C45B-C44B-C43B	117.1(6)
C45B-C44B-C49B	122.6(7)
C43B-C44B-C49B	120.2(7)
C44B-C45B-C46B	121.4(7)
C47B-C46B-C45B	120.1(7)
C46B-C47B-C48B	121.4(7)
C43B-C48B-C47B	116.3(6)
C43B-C48B-C52B	122.3(6)
C47B-C48B-C52B	121.3(6)
C51B-C49B-C44B	112.9(7)
C51B-C49B-C50B	110.5(7)
C44B-C49B-C50B	111.6(6)
C48B-C52B-C54B	112.5(6)
C48B-C52B-C53B	109.4(6)
C54B-C52B-C53B	111.2(6)
C25C-B1C-C1C	109.3(4)
C25C-B1C-C9C	109.1(4)
C1C-B1C-C9C	110.4(4)
C25C-B1C-C17C	111.4(4)
C1C-B1C-C17C	107.5(4)
C9C-B1C-C17C	109.1(4)
C2C-C1C-C6C	115.2(5)

C2C-C1C-B1C	122.1(4)
C6C-C1C-B1C	122.6(4)
C3C-C2C-C1C	122.3(5)
C4C-C3C-C2C	121.5(5)
C4C-C3C-C7C	120.6(5)
C2C-C3C-C7C	118.0(5)
C3C-C4C-C5C	117.5(5)
C4C-C5C-C6C	121.2(5)
C4C-C5C-C8C	119.9(5)
C6C-C5C-C8C	118.9(5)
C5C-C6C-C1C	122.4(5)
F1C-C7C-F2C	106.3(4)
F1C-C7C-F3C	106.4(5)
F2C-C7C-F3C	107.4(4)
F1C-C7C-C3C	112.4(5)
F2C-C7C-C3C	111.2(4)
F3C-C7C-C3C	112.8(5)
F6C-C8C-F4C	105.2(6)
F6C-C8C-F5C	106.7(6)
F4C-C8C-F5C	106.0(6)
F6C-C8C-C5C	113.4(5)
F4C-C8C-C5C	111.8(6)
F5C-C8C-C5C	113.2(5)
C14C-C9C-C10C	116.1(5)
C14C-C9C-B1C	123.3(5)
C10C-C9C-B1C	120.5(5)
C11C-C10C-C9C	122.0(5)
C12C-C11C-C10C	120.4(5)
C12C-C11C-C15C	119.8(5)
C10C-C11C-C15C	119.8(5)
C13C-C12C-C11C	118.7(5)
C12C-C13C-C14C	120.2(5)
C12C-C13C-C16C	120.1(5)
C14C-C13C-C16C	119.6(5)
C9C-C14C-C13C	122.5(5)
F7C-C15C-F8C	106.8(6)
F7C-C15C-F9C	105.4(5)
F8C-C15C-F9C	103.3(5)

F7C-C15C-C11C	114.4(5)
F8C-C15C-C11C	113.4(5)
F9C-C15C-C11C	112.7(5)
F10'-C16C-F12'	109.0(6)
F10C-C16C-F11C	107.9(5)
F10'-C16C-F11'	107.5(6)
F12'-C16C-F11'	105.0(6)
F10C-C16C-F12C	105.3(5)
F11C-C16C-F12C	104.1(5)
F10'-C16C-C13C	111.9(6)
F10C-C16C-C13C	112.6(5)
F12'-C16C-C13C	112.0(6)
F11C-C16C-C13C	113.4(5)
F11'-C16C-C13C	111.1(6)
F12C-C16C-C13C	112.7(5)
C18C-C17C-C22C	115.6(5)
C18C-C17C-B1C	122.3(5)
C22C-C17C-B1C	122.1(5)
C17C-C18C-C19C	122.1(6)
C20C-C19C-C18C	121.1(6)
C20C-C19C-C23C	119.9(6)
C18C-C19C-C23C	118.9(6)
C19C-C20C-C21C	117.7(5)
C22C-C21C-C20C	120.5(5)
C22C-C21C-C24C	119.4(6)
C20C-C21C-C24C	120.1(5)
C21C-C22C-C17C	122.8(5)
F14C-C23C-F15C	106.1(7)
F14C-C23C-F13C	107.2(8)
F15C-C23C-F13C	106.4(8)
F14C-C23C-C19C	111.5(7)
F15C-C23C-C19C	114.2(7)
F13C-C23C-C19C	110.9(7)
F18C-C24C-F17C	107.0(6)
F18C-C24C-F16C	106.6(6)
F17C-C24C-F16C	105.4(5)
F18C-C24C-C21C	112.9(5)
F17C-C24C-C21C	111.7(6)

F16C-C24C-C21C	112.7(6)
C30C-C25C-C26C	115.2(5)
C30C-C25C-B1C	122.9(5)
C26C-C25C-B1C	121.9(4)
C27C-C26C-C25C	122.2(5)
C26C-C27C-C28C	121.1(5)
C26C-C27C-C31C	120.0(5)
C28C-C27C-C31C	118.9(5)
C29C-C28C-C27C	117.5(5)
C28C-C29C-C30C	121.4(5)
C28C-C29C-C32C	118.0(5)
C30C-C29C-C32C	120.5(5)
C29C-C30C-C25C	122.5(5)
F20C-C31C-F21C	107.6(6)
F20C-C31C-F19C	105.4(5)
F21C-C31C-F19C	104.1(5)
F20C-C31C-C27C	114.0(5)
F21C-C31C-C27C	112.0(5)
F19C-C31C-C27C	113.0(5)
F24C-C32C-F23C	106.5(5)
F24C-C32C-F22C	106.8(5)
F23C-C32C-F22C	105.8(4)
F24C-C32C-C29C	113.2(5)
F23C-C32C-C29C	111.7(5)
F22C-C32C-C29C	112.3(5)
C25D-B1D-C17D	111.2(5)
C25D-B1D-C9D	109.9(5)
C17D-B1D-C9D	112.3(5)
C25D-B1D-C1D	107.8(5)
C17D-B1D-C1D	109.0(6)
C9D-B1D-C1D	106.5(5)
C25D-B1D-C1D'	109.5(7)
C17D-B1D-C1D'	100.7(11)
C9D-B1D-C1D'	113.0(9)
C6D-C1D-C2D	117.7(7)
C6D-C1D-B1D	122.8(6)
C2D-C1D-B1D	117.2(6)
C3D-C2D-C1D	120.5(7)

C2D-C3D-C4D	120.8(7)
C2D-C3D-C7D	120.2(7)
C4D-C3D-C7D	119.0(7)
C3D-C4D-C5D	117.7(7)
C6D-C5D-C4D	121.6(6)
C6D-C5D-C8D	119.3(6)
C4D-C5D-C8D	119.1(6)
C1D-C6D-C5D	120.8(6)
F1D-C7D-F2D	99.5(10)
F1D-C7D-F3D	101.8(10)
F2D-C7D-F3D	108.2(11)
F1D-C7D-C3D	113.0(11)
F2D-C7D-C3D	117.9(8)
F3D-C7D-C3D	114.2(9)
F6D-C8D-F4D	109.2(7)
F6D-C8D-F5D	105.1(7)
F4D-C8D-F5D	104.8(7)
F6D-C8D-C5D	113.5(7)
F4D-C8D-C5D	112.0(7)
F5D-C8D-C5D	111.6(7)
C6D'-C1D'-C2D'	116.9(11)
C6D'-C1D'-B1D	118.4(11)
C2D'-C1D'-B1D	115.1(11)
C3D'-C2D'-C1D'	118.9(9)
C4D'-C3D'-C2D'	120.4(8)
C4D'-C3D'-C7D'	119.5(8)
C2D'-C3D'-C7D'	120.0(8)
C3D'-C4D'-C5D'	118.3(8)
C6D'-C5D'-C4D'	120.8(8)
C6D'-C5D'-C8D'	119.1(7)
C4D'-C5D'-C8D'	120.1(7)
C1D'-C6D'-C5D'	119.3(8)
F1D'-C7D'-F2D'	99.5(12)
F1D'-C7D'-F3D'	101.3(11)
F2D'-C7D'-F3D'	109.9(12)
F1D'-C7D'-C3D'	113.7(12)
F2D'-C7D'-C3D'	116.4(9)
F3D'-C7D'-C3D'	114.2(10)

F6D'-C8D'-F4D'	109.2(10)
F6D'-C8D'-F5D'	104.9(10)
F4D'-C8D'-F5D'	104.1(9)
F6D'-C8D'-C5D'	113.4(9)
F4D'-C8D'-C5D'	112.7(9)
F5D'-C8D'-C5D'	111.9(10)
C10D-C9D-C14D	115.0(5)
C10D-C9D-B1D	123.4(5)
C14D-C9D-B1D	121.6(6)
C11D-C10D-C9D	123.4(6)
C12D-C11D-C10D	120.3(6)
C12D-C11D-C15D	118.1(6)
C10D-C11D-C15D	121.6(6)
C11D-C12D-C13D	118.5(6)
C12D-C13D-C14D	120.3(6)
C12D-C13D-C16D	120.3(6)
C14D-C13D-C16D	119.4(6)
C13D-C14D-C9D	122.5(6)
F9D-C15D-F8D	105.6(5)
F9D-C15D-F7D	105.7(6)
F8D-C15D-F7D	105.2(6)
F9D-C15D-C11D	113.4(6)
F8D-C15D-C11D	113.0(6)
F7D-C15D-C11D	113.2(5)
F10D-C16D-F12D	107.5(7)
F10D-C16D-F11D	104.0(5)
F12D-C16D-F11D	104.1(6)
F10D-C16D-C13D	115.3(6)
F12D-C16D-C13D	113.5(6)
F11D-C16D-C13D	111.4(7)
C18D-C17D-C22D	114.3(6)
C18D-C17D-B1D	119.9(5)
C22D-C17D-B1D	125.8(6)
C19D-C18D-C17D	122.7(6)
C20D-C19D-C18D	120.2(7)
C20D-C19D-C23D	120.9(7)
C18D-C19D-C23D	118.8(6)
C21D-C20D-C19D	118.5(7)

C20D-C21D-C22D	121.3(6)
C20D-C21D-C24D	119.2(7)
C22D-C21D-C24D	119.5(7)
C21D-C22D-C17D	122.9(6)
F13D-C23D-F14D	107.8(7)
F13D-C23D-F15D	104.9(8)
F14D-C23D-F15D	108.1(8)
F13D-C23D-C19D	112.6(8)
F14D-C23D-C19D	111.7(7)
F15D-C23D-C19D	111.3(7)
F18D-C24D-F17D	106.0(7)
F18D-C24D-F16D	105.3(7)
F17D-C24D-F16D	105.5(7)
F18D-C24D-C21D	111.9(7)
F17D-C24D-C21D	114.3(7)
F16D-C24D-C21D	113.1(6)
C30D-C25D-C26D	114.6(6)
C30D-C25D-B1D	122.4(5)
C26D-C25D-B1D	122.7(5)
C27D-C26D-C25D	122.7(6)
C28D-C27D-C26D	121.3(5)
C28D-C27D-C31D	119.5(5)
C26D-C27D-C31D	119.2(5)
C27D-C28D-C29D	117.1(6)
C30D-C29D-C28D	120.6(6)
C30D-C29D-C32D	119.8(6)
C28D-C29D-C32D	119.5(6)
C29D-C30D-C25D	123.7(6)
F20D-C31D-F19D	106.7(5)
F20D-C31D-F21D	106.1(5)
F19D-C31D-F21D	106.5(5)
F20D-C31D-C27D	111.8(5)
F19D-C31D-C27D	112.1(5)
F21D-C31D-C27D	113.2(5)
F22D-C32D-F24D	105.1(7)
F22D-C32D-F23D	108.0(7)
F24D-C32D-F23D	100.9(7)
F22D-C32D-C29D	115.7(6)

F24D-C32D-C29D	113.6(6)
F23D-C32D-C29D	112.4(7)

Table 3. Torsion angles [°] for SFC-A-94.

C3A-N2A-C1A-N1A	0.6(7)
C16A-N2A-C1A-N1A	179.6(5)
C3A-N2A-C1A-Au1A	177.9(4)
C16A-N2A-C1A-Au1A	-3.0(9)
C2A-N1A-C1A-N2A	0.0(7)
C4A-N1A-C1A-N2A	-178.5(5)
C2A-N1A-C1A-Au1A	-177.3(4)
C4A-N1A-C1A-Au1A	4.1(9)
C1A-N1A-C2A-C3A	-0.6(7)
C4A-N1A-C2A-C3A	178.0(5)
N1A-C2A-C3A-N2A	0.9(7)
C1A-N2A-C3A-C2A	-0.9(7)
C16A-N2A-C3A-C2A	179.9(5)
C1A-N1A-C4A-C9A	-105.1(7)
C2A-N1A-C4A-C9A	76.5(7)
C1A-N1A-C4A-C5A	80.5(7)
C2A-N1A-C4A-C5A	-97.8(7)
C9A-C4A-C5A-C6A	1.6(8)
N1A-C4A-C5A-C6A	175.6(5)
C9A-C4A-C5A-C10A	-173.6(5)
N1A-C4A-C5A-C10A	0.5(8)
C4A-C5A-C6A-C7A	-2.1(9)
C10A-C5A-C6A-C7A	173.1(6)
C5A-C6A-C7A-C8A	1.9(10)
C6A-C7A-C8A-C9A	-1.0(10)
C5A-C4A-C9A-C8A	-0.8(8)
N1A-C4A-C9A-C8A	-174.8(5)
C5A-C4A-C9A-C13A	178.7(5)
N1A-C4A-C9A-C13A	4.7(8)
C7A-C8A-C9A-C4A	0.5(9)
C7A-C8A-C9A-C13A	-179.0(6)
C6A-C5A-C10A-C12A	-89.6(7)
C4A-C5A-C10A-C12A	85.4(7)

C6A-C5A-C10A-C11A	31.3(8)
C4A-C5A-C10A-C11A	-153.7(6)
C4A-C9A-C13A-C14A	84.2(8)
C8A-C9A-C13A-C14A	-96.3(8)
C4A-C9A-C13A-C15A	-149.1(6)
C8A-C9A-C13A-C15A	30.4(9)
C1A-N2A-C16A-C17A	96.6(7)
C3A-N2A-C16A-C17A	-84.4(7)
C1A-N2A-C16A-C21A	-89.0(7)
C3A-N2A-C16A-C21A	89.9(7)
C21A-C16A-C17A-C18A	1.1(8)
N2A-C16A-C17A-C18A	175.1(5)
C21A-C16A-C17A-C22A	-178.2(5)
N2A-C16A-C17A-C22A	-4.1(8)
C16A-C17A-C18A-C19A	-0.9(8)
C22A-C17A-C18A-C19A	178.4(5)
C17A-C18A-C19A-C20A	0.5(9)
C18A-C19A-C20A-C21A	-0.3(9)
C17A-C16A-C21A-C20A	-0.8(8)
N2A-C16A-C21A-C20A	-174.8(5)
C17A-C16A-C21A-C25A	177.3(5)
N2A-C16A-C21A-C25A	3.3(8)
C19A-C20A-C21A-C16A	0.4(8)
C19A-C20A-C21A-C25A	-177.8(5)
C16A-C17A-C22A-C24A	142.2(6)
C18A-C17A-C22A-C24A	-37.0(7)
C16A-C17A-C22A-C23A	-94.9(7)
C18A-C17A-C22A-C23A	85.9(7)
C16A-C21A-C25A-C26A	-101.0(8)
C20A-C21A-C25A-C26A	77.0(8)
C16A-C21A-C25A-C27A	136.7(6)
C20A-C21A-C25A-C27A	-45.2(8)
C30A-N4A-C28A-N3A	-2.1(6)
C43A-N4A-C28A-N3A	178.5(5)
C30A-N4A-C28A-Au1A	176.4(4)
C43A-N4A-C28A-Au1A	-2.9(9)
C29A-N3A-C28A-N4A	1.7(6)
C31A-N3A-C28A-N4A	-170.1(5)

C29A-N3A-C28A-Au1A	-176.9(4)
C31A-N3A-C28A-Au1A	11.3(8)
C28A-N3A-C29A-C30A	-0.7(7)
C31A-N3A-C29A-C30A	171.6(5)
N3A-C29A-C30A-N4A	-0.7(6)
C28A-N4A-C30A-C29A	1.8(7)
C43A-N4A-C30A-C29A	-178.8(5)
C28A-N3A-C31A-C32A	-100.6(7)
C29A-N3A-C31A-C32A	88.2(7)
C28A-N3A-C31A-C36A	86.0(7)
C29A-N3A-C31A-C36A	-85.1(7)
C36A-C31A-C32A-C33A	-0.7(9)
N3A-C31A-C32A-C33A	-173.7(5)
C36A-C31A-C32A-C37A	178.5(6)
N3A-C31A-C32A-C37A	5.5(8)
C31A-C32A-C33A-C34A	0.8(9)
C37A-C32A-C33A-C34A	-178.4(6)
C32A-C33A-C34A-C35A	-0.2(10)
C33A-C34A-C35A-C36A	-0.7(10)
C34A-C35A-C36A-C31A	0.9(9)
C34A-C35A-C36A-C40A	-178.3(6)
C32A-C31A-C36A-C35A	-0.2(9)
N3A-C31A-C36A-C35A	172.8(5)
C32A-C31A-C36A-C40A	179.1(6)
N3A-C31A-C36A-C40A	-8.0(8)
C31A-C32A-C37A-C38A	93.0(11)
C33A-C32A-C37A-C38A	-87.8(11)
C31A-C32A-C37A-C39'	-122.0(12)
C33A-C32A-C37A-C39'	57.2(13)
C31A-C32A-C37A-C39A	-134.8(11)
C33A-C32A-C37A-C39A	44.4(12)
C31A-C32A-C37A-C38'	117.8(9)
C33A-C32A-C37A-C38'	-63.1(10)
C35A-C36A-C40A-C41A	-46.8(8)
C31A-C36A-C40A-C41A	134.0(7)
C35A-C36A-C40A-C42A	77.6(7)
C31A-C36A-C40A-C42A	-101.6(7)
C28A-N4A-C43A-C48A	101.8(7)

C30A-N4A-C43A-C48A	-77.5(7)
C28A-N4A-C43A-C44A	-84.4(7)
C30A-N4A-C43A-C44A	96.3(7)
C48A-C43A-C44A-C45A	0.6(9)
N4A-C43A-C44A-C45A	-172.8(5)
C48A-C43A-C44A-C49A	-179.3(6)
N4A-C43A-C44A-C49A	7.3(8)
C43A-C44A-C45A-C46A	0.1(9)
C49A-C44A-C45A-C46A	180.0(6)
C44A-C45A-C46A-C47A	-0.4(10)
C45A-C46A-C47A-C48A	0.1(9)
C44A-C43A-C48A-C47A	-0.9(9)
N4A-C43A-C48A-C47A	172.5(5)
C44A-C43A-C48A-C52A	176.2(5)
N4A-C43A-C48A-C52A	-10.4(8)
C46A-C47A-C48A-C43A	0.5(9)
C46A-C47A-C48A-C52A	-176.6(6)
C45A-C44A-C49A-C51A	-26.0(9)
C43A-C44A-C49A-C51A	153.8(6)
C45A-C44A-C49A-C50A	99.5(7)
C43A-C44A-C49A-C50A	-80.6(7)
C43A-C48A-C52A-C54A	-88.8(7)
C47A-C48A-C52A-C54A	88.1(7)
C43A-C48A-C52A-C53A	146.8(6)
C47A-C48A-C52A-C53A	-36.2(8)
C2B-N1B-C1B-N2B	-1.4(6)
C4B-N1B-C1B-N2B	-175.1(4)
C2B-N1B-C1B-Au1B	-176.1(4)
C4B-N1B-C1B-Au1B	10.2(7)
C3B-N2B-C1B-N1B	1.1(6)
C16B-N2B-C1B-N1B	173.2(5)
C3B-N2B-C1B-Au1B	176.0(4)
C16B-N2B-C1B-Au1B	-11.9(8)
C1B-N1B-C2B-C3B	1.3(6)
C4B-N1B-C2B-C3B	175.4(4)
N1B-C2B-C3B-N2B	-0.6(6)
C1B-N2B-C3B-C2B	-0.3(6)
C16B-N2B-C3B-C2B	-173.0(5)

C1B-N1B-C4B-C9B	85.6(7)
C2B-N1B-C4B-C9B	-87.5(6)
C1B-N1B-C4B-C5B	-99.9(6)
C2B-N1B-C4B-C5B	86.9(6)
C9B-C4B-C5B-C6B	-4.6(8)
N1B-C4B-C5B-C6B	-178.7(5)
C9B-C4B-C5B-C10B	173.7(5)
N1B-C4B-C5B-C10B	-0.4(8)
C4B-C5B-C6B-C7B	1.3(9)
C10B-C5B-C6B-C7B	-177.0(5)
C5B-C6B-C7B-C8B	1.7(9)
C6B-C7B-C8B-C9B	-1.5(9)
C5B-C4B-C9B-C8B	4.7(8)
N1B-C4B-C9B-C8B	178.9(5)
C5B-C4B-C9B-C13B	-175.2(5)
N1B-C4B-C9B-C13B	-1.0(8)
C7B-C8B-C9B-C4B	-1.5(9)
C7B-C8B-C9B-C13B	178.4(5)
C6B-C5B-C10B-C11B	-96.0(7)
C4B-C5B-C10B-C11B	85.8(7)
C6B-C5B-C10B-C12B	27.9(8)
C4B-C5B-C10B-C12B	-150.3(6)
C4B-C9B-C13B-C14"	-134.2(11)
C8B-C9B-C13B-C14"	45.9(12)
C4B-C9B-C13B-C15B	131.9(7)
C8B-C9B-C13B-C15B	-48.1(8)
C4B-C9B-C13B-C14B	-104.5(7)
C8B-C9B-C13B-C14B	75.5(7)
C4B-C9B-C13B-C15"	103.4(11)
C8B-C9B-C13B-C15"	-76.5(12)
C1B-N2B-C16B-C21B	108.0(6)
C3B-N2B-C16B-C21B	-80.7(7)
C1B-N2B-C16B-C17B	-77.9(7)
C3B-N2B-C16B-C17B	93.4(6)
C21B-C16B-C17B-C18B	1.5(9)
N2B-C16B-C17B-C18B	-172.3(5)
C21B-C16B-C17B-C22B	179.3(5)
N2B-C16B-C17B-C22B	5.5(8)

C16B-C17B-C18B-C19B	0.8(9)
C22B-C17B-C18B-C19B	-177.1(5)
C17B-C18B-C19B-C20B	-1.8(10)
C18B-C19B-C20B-C21B	0.5(10)
C17B-C16B-C21B-C20B	-2.7(9)
N2B-C16B-C21B-C20B	171.0(5)
C17B-C16B-C21B-C25B	177.8(6)
N2B-C16B-C21B-C25B	-8.5(9)
C19B-C20B-C21B-C16B	1.7(10)
C19B-C20B-C21B-C25B	-178.8(6)
C18B-C17B-C22B-C23B	-61.3(9)
C16B-C17B-C22B-C23B	120.9(8)
C18B-C17B-C22B-C24"	86.7(10)
C16B-C17B-C22B-C24"	-91.0(10)
C18B-C17B-C22B-C24B	63.9(9)
C16B-C17B-C22B-C24B	-113.9(8)
C18B-C17B-C22B-C23"	-35.7(10)
C16B-C17B-C22B-C23"	146.6(9)
C16B-C21B-C25B-C27B	-129.7(7)
C20B-C21B-C25B-C27B	50.8(8)
C16B-C21B-C25B-C26B	107.3(7)
C20B-C21B-C25B-C26B	-72.2(8)
C29B-N3B-C28B-N4B	-0.4(8)
C31B-N3B-C28B-N4B	171.8(7)
C29B-N3B-C28B-Au1B	173.6(6)
C31B-N3B-C28B-Au1B	-14.2(11)
C30B-N4B-C28B-N3B	-0.5(8)
C43B-N4B-C28B-N3B	-177.9(6)
C30B-N4B-C28B-Au1B	-174.3(6)
C43B-N4B-C28B-Au1B	8.3(11)
C28B-N3B-C29B-C30B	1.2(10)
C31B-N3B-C29B-C30B	-171.5(7)
N3B-C29B-C30B-N4B	-1.4(10)
C28B-N4B-C30B-C29B	1.3(10)
C43B-N4B-C30B-C29B	178.8(7)
C28B-N3B-C31B-C36B	-79.8(9)
C29B-N3B-C31B-C36B	91.7(8)
C28B-N3B-C31B-C32B	108.2(8)

C29B-N3B-C31B-C32B	-80.3(9)
C36B-C31B-C32B-C33B	2.0(9)
N3B-C31B-C32B-C33B	173.6(6)
C36B-C31B-C32B-C37B	-177.5(6)
N3B-C31B-C32B-C37B	-6.0(9)
C31B-C32B-C33B-C34B	-1.0(10)
C37B-C32B-C33B-C34B	178.5(7)
C32B-C33B-C34B-C35B	0.2(11)
C33B-C34B-C35B-C36B	-0.4(11)
C34B-C35B-C36B-C31B	1.3(10)
C34B-C35B-C36B-C40B	-178.2(6)
C32B-C31B-C36B-C35B	-2.2(9)
N3B-C31B-C36B-C35B	-173.8(6)
C32B-C31B-C36B-C40B	177.3(6)
N3B-C31B-C36B-C40B	5.6(9)
C33B-C32B-C37B-C38B	100.0(8)
C31B-C32B-C37B-C38B	-80.4(8)
C33B-C32B-C37B-C39B	-21.8(9)
C31B-C32B-C37B-C39B	157.7(6)
C35B-C36B-C40B-C41B	48.2(9)
C31B-C36B-C40B-C41B	-131.3(7)
C35B-C36B-C40B-C42B	-75.1(8)
C31B-C36B-C40B-C42B	105.4(7)
C28B-N4B-C43B-C48B	-107.1(8)
C30B-N4B-C43B-C48B	75.8(8)
C28B-N4B-C43B-C44B	79.1(9)
C30B-N4B-C43B-C44B	-98.1(8)
C48B-C43B-C44B-C45B	0.8(10)
N4B-C43B-C44B-C45B	174.2(6)
C48B-C43B-C44B-C49B	-179.0(6)
N4B-C43B-C44B-C49B	-5.6(9)
C43B-C44B-C45B-C46B	-2.4(10)
C49B-C44B-C45B-C46B	177.4(7)
C44B-C45B-C46B-C47B	2.5(11)
C45B-C46B-C47B-C48B	-0.8(11)
C44B-C43B-C48B-C47B	0.7(9)
N4B-C43B-C48B-C47B	-172.9(5)
C44B-C43B-C48B-C52B	-176.1(6)

N4B-C43B-C48B-C52B	10.3(9)
C46B-C47B-C48B-C43B	-0.7(10)
C46B-C47B-C48B-C52B	176.1(6)
C45B-C44B-C49B-C51B	24.1(10)
C43B-C44B-C49B-C51B	-156.1(7)
C45B-C44B-C49B-C50B	-101.2(9)
C43B-C44B-C49B-C50B	78.6(9)
C43B-C48B-C52B-C54B	-141.6(6)
C47B-C48B-C52B-C54B	41.8(9)
C43B-C48B-C52B-C53B	94.3(7)
C47B-C48B-C52B-C53B	-82.3(8)
C25C-B1C-C1C-C2C	39.1(6)
C9C-B1C-C1C-C2C	159.1(5)
C17C-B1C-C1C-C2C	-82.0(6)
C25C-B1C-C1C-C6C	-144.1(5)
C9C-B1C-C1C-C6C	-24.1(7)
C17C-B1C-C1C-C6C	94.8(6)
C6C-C1C-C2C-C3C	-0.1(8)
B1C-C1C-C2C-C3C	176.9(5)
C1C-C2C-C3C-C4C	0.8(8)
C1C-C2C-C3C-C7C	-178.8(5)
C2C-C3C-C4C-C5C	-1.0(8)
C7C-C3C-C4C-C5C	178.6(5)
C3C-C4C-C5C-C6C	0.5(8)
C3C-C4C-C5C-C8C	-178.5(6)
C4C-C5C-C6C-C1C	0.2(9)
C8C-C5C-C6C-C1C	179.2(6)
C2C-C1C-C6C-C5C	-0.4(8)
B1C-C1C-C6C-C5C	-177.4(5)
C4C-C3C-C7C-F1C	119.3(6)
C2C-C3C-C7C-F1C	-61.0(7)
C4C-C3C-C7C-F2C	-121.6(6)
C2C-C3C-C7C-F2C	58.0(7)
C4C-C3C-C7C-F3C	-0.9(7)
C2C-C3C-C7C-F3C	178.7(5)
C4C-C5C-C8C-F6C	-148.3(6)
C6C-C5C-C8C-F6C	32.7(9)
C4C-C5C-C8C-F4C	93.0(7)

C6C-C5C-C8C-F4C	-85.9(7)
C4C-C5C-C8C-F5C	-26.6(9)
C6C-C5C-C8C-F5C	154.5(6)
C25C-B1C-C9C-C14C	-102.9(6)
C1C-B1C-C9C-C14C	136.9(5)
C17C-B1C-C9C-C14C	19.0(7)
C25C-B1C-C9C-C10C	72.8(6)
C1C-B1C-C9C-C10C	-47.4(6)
C17C-B1C-C9C-C10C	-165.2(5)
C14C-C9C-C10C-C11C	2.5(7)
B1C-C9C-C10C-C11C	-173.6(5)
C9C-C10C-C11C-C12C	-1.7(8)
C9C-C10C-C11C-C15C	179.5(5)
C10C-C11C-C12C-C13C	-0.1(8)
C15C-C11C-C12C-C13C	178.7(5)
C11C-C12C-C13C-C14C	1.0(8)
C11C-C12C-C13C-C16C	-177.2(5)
C10C-C9C-C14C-C13C	-1.6(8)
B1C-C9C-C14C-C13C	174.3(5)
C12C-C13C-C14C-C9C	-0.1(8)
C16C-C13C-C14C-C9C	178.1(5)
C12C-C11C-C15C-F7C	152.7(6)
C10C-C11C-C15C-F7C	-28.4(8)
C12C-C11C-C15C-F8C	-84.5(7)
C10C-C11C-C15C-F8C	94.3(7)
C12C-C11C-C15C-F9C	32.4(8)
C10C-C11C-C15C-F9C	-148.8(5)
C12C-C13C-C16C-F10'	-106.2(7)
C14C-C13C-C16C-F10'	75.6(7)
C12C-C13C-C16C-F10C	103.3(6)
C14C-C13C-C16C-F10C	-74.9(7)
C12C-C13C-C16C-F12'	131.1(7)
C14C-C13C-C16C-F12'	-47.1(8)
C12C-C13C-C16C-F11C	-19.6(8)
C14C-C13C-C16C-F11C	162.2(6)
C12C-C13C-C16C-F11'	13.9(8)
C14C-C13C-C16C-F11'	-164.3(6)
C12C-C13C-C16C-F12C	-137.6(6)

C14C-C13C-C16C-F12C	44.2(7)
C25C-B1C-C17C-C18C	28.6(7)
C1C-B1C-C17C-C18C	148.4(5)
C9C-B1C-C17C-C18C	-91.9(6)
C25C-B1C-C17C-C22C	-154.0(5)
C1C-B1C-C17C-C22C	-34.2(6)
C9C-B1C-C17C-C22C	85.5(6)
C22C-C17C-C18C-C19C	3.1(8)
B1C-C17C-C18C-C19C	-179.4(5)
C17C-C18C-C19C-C20C	-3.4(9)
C17C-C18C-C19C-C23C	175.2(6)
C18C-C19C-C20C-C21C	1.1(9)
C23C-C19C-C20C-C21C	-177.4(6)
C19C-C20C-C21C-C22C	1.1(8)
C19C-C20C-C21C-C24C	179.9(6)
C20C-C21C-C22C-C17C	-1.3(8)
C24C-C21C-C22C-C17C	179.9(5)
C18C-C17C-C22C-C21C	-0.8(7)
B1C-C17C-C22C-C21C	-178.4(5)
C20C-C19C-C23C-F14C	-113.1(8)
C18C-C19C-C23C-F14C	68.3(9)
C20C-C19C-C23C-F15C	7.1(11)
C18C-C19C-C23C-F15C	-171.5(6)
C20C-C19C-C23C-F13C	127.4(8)
C18C-C19C-C23C-F13C	-51.2(11)
C22C-C21C-C24C-F18C	-47.9(8)
C20C-C21C-C24C-F18C	133.2(6)
C22C-C21C-C24C-F17C	72.7(7)
C20C-C21C-C24C-F17C	-106.1(7)
C22C-C21C-C24C-F16C	-168.8(5)
C20C-C21C-C24C-F16C	12.3(8)
C1C-B1C-C25C-C30C	-82.8(6)
C9C-B1C-C25C-C30C	156.3(5)
C17C-B1C-C25C-C30C	35.8(7)
C1C-B1C-C25C-C26C	96.0(6)
C9C-B1C-C25C-C26C	-24.9(7)
C17C-B1C-C25C-C26C	-145.4(5)
C30C-C25C-C26C-C27C	1.1(8)

B1C-C25C-C26C-C27C	-177.8(5)
C25C-C26C-C27C-C28C	-2.0(9)
C25C-C26C-C27C-C31C	179.4(5)
C26C-C27C-C28C-C29C	1.2(9)
C31C-C27C-C28C-C29C	179.8(5)
C27C-C28C-C29C-C30C	0.4(8)
C27C-C28C-C29C-C32C	-176.5(5)
C28C-C29C-C30C-C25C	-1.3(8)
C32C-C29C-C30C-C25C	175.6(5)
C26C-C25C-C30C-C29C	0.6(8)
B1C-C25C-C30C-C29C	179.5(5)
C26C-C27C-C31C-F20C	-4.4(9)
C28C-C27C-C31C-F20C	177.0(6)
C26C-C27C-C31C-F21C	-126.9(6)
C28C-C27C-C31C-F21C	54.5(8)
C26C-C27C-C31C-F19C	116.0(6)
C28C-C27C-C31C-F19C	-62.7(7)
C28C-C29C-C32C-F24C	-169.1(5)
C30C-C29C-C32C-F24C	13.9(7)
C28C-C29C-C32C-F23C	70.7(7)
C30C-C29C-C32C-F23C	-106.3(6)
C28C-C29C-C32C-F22C	-48.0(7)
C30C-C29C-C32C-F22C	135.0(5)
C25D-B1D-C1D-C6D	-150.5(14)
C17D-B1D-C1D-C6D	88.7(14)
C9D-B1D-C1D-C6D	-32.6(16)
C25D-B1D-C1D-C2D	47.3(12)
C17D-B1D-C1D-C2D	-73.5(11)
C9D-B1D-C1D-C2D	165.2(9)
C6D-C1D-C2D-C3D	11.3(19)
B1D-C1D-C2D-C3D	174.4(9)
C1D-C2D-C3D-C4D	-9.2(17)
C1D-C2D-C3D-C7D	171.2(11)
C2D-C3D-C4D-C5D	3.9(16)
C7D-C3D-C4D-C5D	-176.5(11)
C3D-C4D-C5D-C6D	-1(2)
C3D-C4D-C5D-C8D	-178.6(10)
C2D-C1D-C6D-C5D	-9(3)

B1D-C1D-C6D-C5D	-170.6(18)
C4D-C5D-C6D-C1D	4(3)
C8D-C5D-C6D-C1D	-178.8(15)
C2D-C3D-C7D-F1D	69.2(14)
C4D-C3D-C7D-F1D	-110.4(13)
C2D-C3D-C7D-F2D	-46.2(17)
C4D-C3D-C7D-F2D	134.2(12)
C2D-C3D-C7D-F3D	-175.0(11)
C4D-C3D-C7D-F3D	5.4(16)
C6D-C5D-C8D-F6D	45.4(19)
C4D-C5D-C8D-F6D	-137.0(12)
C6D-C5D-C8D-F4D	-78.9(18)
C4D-C5D-C8D-F4D	98.7(12)
C6D-C5D-C8D-F5D	163.9(17)
C4D-C5D-C8D-F5D	-18.4(14)
C25D-B1D-C1D'-C6D'	-140(3)
C17D-B1D-C1D'-C6D'	103(3)
C9D-B1D-C1D'-C6D'	-17(3)
C25D-B1D-C1D'-C2D'	5(3)
C17D-B1D-C1D'-C2D'	-112(2)
C9D-B1D-C1D'-C2D'	128(2)
C6D'-C1D'-C2D'-C3D'	-26(3)
B1D-C1D'-C2D'-C3D'	-172.2(19)
C1D'-C2D'-C3D'-C4D'	14(4)
C1D'-C2D'-C3D'-C7D'	-163(2)
C2D'-C3D'-C4D'-C5D'	0(4)
C7D'-C3D'-C4D'-C5D'	177(2)
C3D'-C4D'-C5D'-C6D'	-1(5)
C3D'-C4D'-C5D'-C8D'	177(2)
C2D'-C1D'-C6D'-C5D'	26(5)
B1D-C1D'-C6D'-C5D'	170(4)
C4D'-C5D'-C6D'-C1D'	-12(7)
C8D'-C5D'-C6D'-C1D'	170(3)
C4D'-C3D'-C7D'-F1D'	128(2)
C2D'-C3D'-C7D'-F1D'	-55(2)
C4D'-C3D'-C7D'-F2D'	13(3)
C2D'-C3D'-C7D'-F2D'	-170(2)
C4D'-C3D'-C7D'-F3D'	-117(2)

C2D'-C3D'-C7D'-F3D'	60(2)
C6D'-C5D'-C8D'-F6D'	162(4)
C4D'-C5D'-C8D'-F6D'	-16(3)
C6D'-C5D'-C8D'-F4D'	37(4)
C4D'-C5D'-C8D'-F4D'	-141(3)
C6D'-C5D'-C8D'-F5D'	-80(4)
C4D'-C5D'-C8D'-F5D'	102(3)
C25D-B1D-C9D-C10D	19.7(7)
C17D-B1D-C9D-C10D	144.0(6)
C1D-B1D-C9D-C10D	-96.9(8)
C1D'-B1D-C9D-C10D	-103.0(11)
C25D-B1D-C9D-C14D	-159.7(5)
C17D-B1D-C9D-C14D	-35.4(7)
C1D-B1D-C9D-C14D	83.8(8)
C1D'-B1D-C9D-C14D	77.6(12)
C14D-C9D-C10D-C11D	-0.4(9)
B1D-C9D-C10D-C11D	-179.8(5)
C9D-C10D-C11D-C12D	0.3(9)
C9D-C10D-C11D-C15D	-178.5(6)
C10D-C11D-C12D-C13D	-0.5(9)
C15D-C11D-C12D-C13D	178.3(6)
C11D-C12D-C13D-C14D	0.8(9)
C11D-C12D-C13D-C16D	178.4(6)
C12D-C13D-C14D-C9D	-1.0(9)
C16D-C13D-C14D-C9D	-178.6(6)
C10D-C9D-C14D-C13D	0.8(9)
B1D-C9D-C14D-C13D	-179.8(5)
C12D-C11D-C15D-F9D	47.7(8)
C10D-C11D-C15D-F9D	-133.5(6)
C12D-C11D-C15D-F8D	-72.5(8)
C10D-C11D-C15D-F8D	106.3(7)
C12D-C11D-C15D-F7D	168.1(6)
C10D-C11D-C15D-F7D	-13.1(9)
C12D-C13D-C16D-F10D	152.7(6)
C14D-C13D-C16D-F10D	-29.7(9)
C12D-C13D-C16D-F12D	-82.6(9)
C14D-C13D-C16D-F12D	95.0(8)
C12D-C13D-C16D-F11D	34.5(9)

C14D-C13D-C16D-F11D	-147.9(6)
C25D-B1D-C17D-C18D	83.0(6)
C9D-B1D-C17D-C18D	-40.6(7)
C1D-B1D-C17D-C18D	-158.3(5)
C1D'-B1D-C17D-C18D	-161.0(7)
C25D-B1D-C17D-C22D	-92.4(7)
C9D-B1D-C17D-C22D	144.0(6)
C1D-B1D-C17D-C22D	26.4(8)
C1D'-B1D-C17D-C22D	23.6(9)
C22D-C17D-C18D-C19D	2.9(9)
B1D-C17D-C18D-C19D	-173.0(6)
C17D-C18D-C19D-C20D	-3.4(10)
C17D-C18D-C19D-C23D	173.0(7)
C18D-C19D-C20D-C21D	2.6(10)
C23D-C19D-C20D-C21D	-173.8(7)
C19D-C20D-C21D-C22D	-1.5(10)
C19D-C20D-C21D-C24D	-178.5(6)
C20D-C21D-C22D-C17D	1.2(10)
C24D-C21D-C22D-C17D	178.2(6)
C18D-C17D-C22D-C21D	-1.8(9)
B1D-C17D-C22D-C21D	173.8(6)
C20D-C19D-C23D-F13D	-143.5(7)
C18D-C19D-C23D-F13D	40.1(10)
C20D-C19D-C23D-F14D	-22.0(11)
C18D-C19D-C23D-F14D	161.6(7)
C20D-C19D-C23D-F15D	99.0(8)
C18D-C19D-C23D-F15D	-77.4(9)
C20D-C21D-C24D-F18D	-128.6(8)
C22D-C21D-C24D-F18D	54.3(9)
C20D-C21D-C24D-F17D	-8.2(10)
C22D-C21D-C24D-F17D	174.7(7)
C20D-C21D-C24D-F16D	112.6(8)
C22D-C21D-C24D-F16D	-64.5(10)
C17D-B1D-C25D-C30D	163.6(5)
C9D-B1D-C25D-C30D	-71.5(7)
C1D-B1D-C25D-C30D	44.1(8)
C1D'-B1D-C25D-C30D	53.2(13)
C17D-B1D-C25D-C26D	-23.3(7)

C9D-B1D-C25D-C26D	101.6(6)
C1D-B1D-C25D-C26D	-142.7(6)
C1D'-B1D-C25D-C26D	-133.7(12)
C30D-C25D-C26D-C27D	0.4(8)
B1D-C25D-C26D-C27D	-173.2(5)
C25D-C26D-C27D-C28D	1.2(9)
C25D-C26D-C27D-C31D	-179.1(5)
C26D-C27D-C28D-C29D	-1.6(8)
C31D-C27D-C28D-C29D	178.7(5)
C27D-C28D-C29D-C30D	0.4(9)
C27D-C28D-C29D-C32D	179.1(6)
C28D-C29D-C30D-C25D	1.3(10)
C32D-C29D-C30D-C25D	-177.4(6)
C26D-C25D-C30D-C29D	-1.7(9)
B1D-C25D-C30D-C29D	172.0(6)
C28D-C27D-C31D-F20D	-117.7(6)
C26D-C27D-C31D-F20D	62.6(7)
C28D-C27D-C31D-F19D	122.6(6)
C26D-C27D-C31D-F19D	-57.1(7)
C28D-C27D-C31D-F21D	2.1(8)
C26D-C27D-C31D-F21D	-177.6(5)
C30D-C29D-C32D-F22D	175.4(7)
C28D-C29D-C32D-F22D	-3.4(10)
C30D-C29D-C32D-F24D	53.7(10)
C28D-C29D-C32D-F24D	-125.1(7)
C30D-C29D-C32D-F23D	-60.0(9)
C28D-C29D-C32D-F23D	121.2(8)

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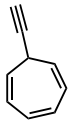
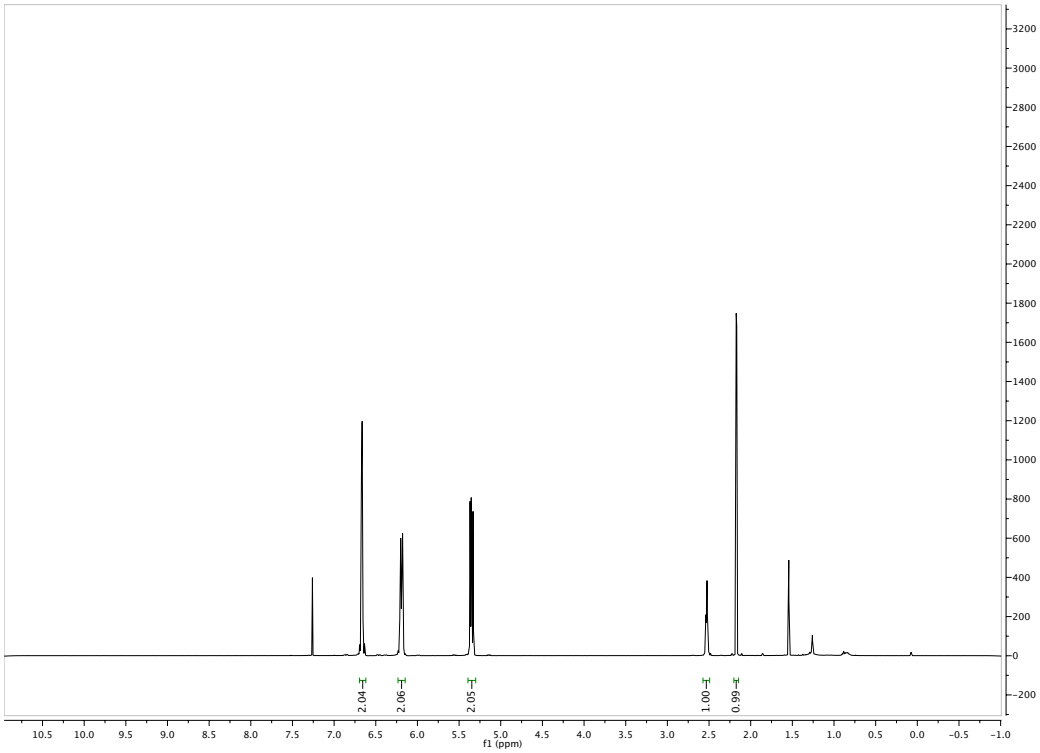
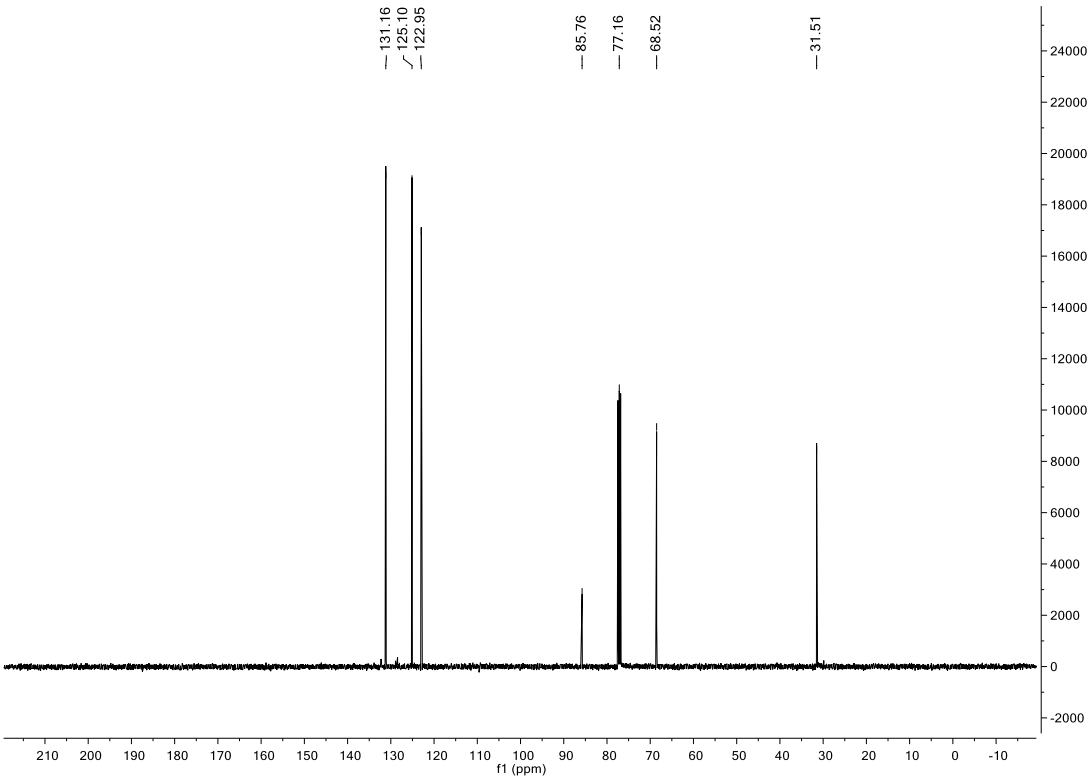
5. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR, ^{31}P NMR, ^{11}B NMR spectra

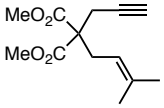
7-Ethynylcyclohepta-1,3,5-triene (11)

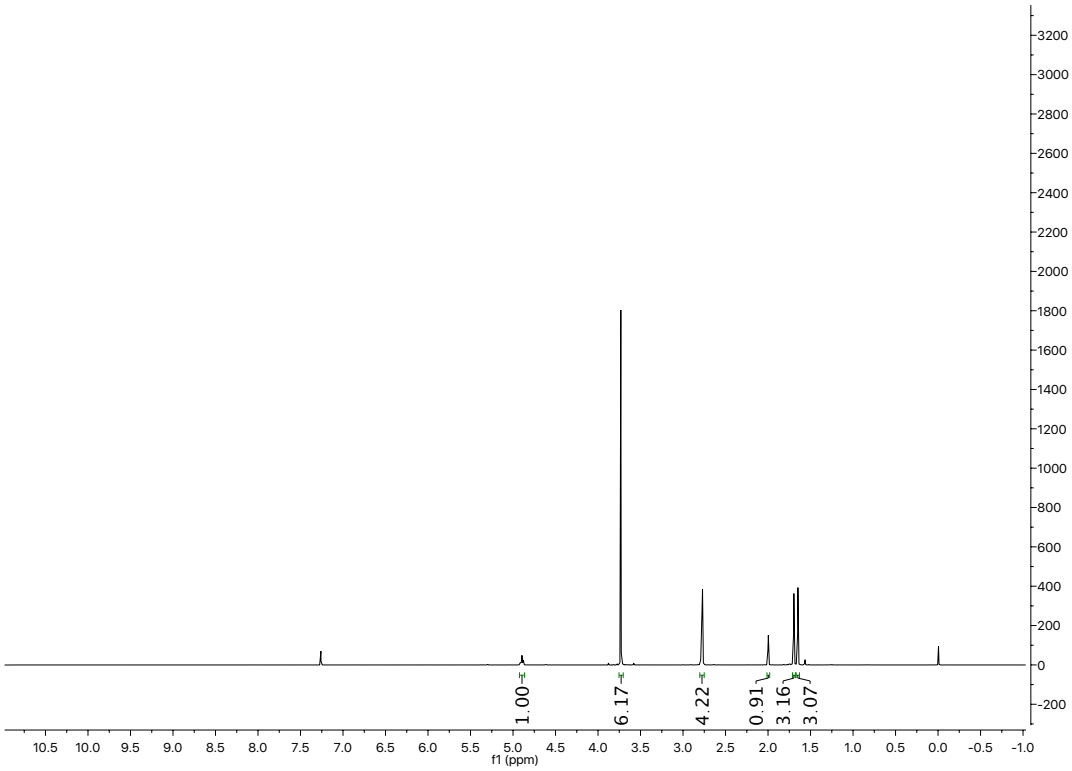


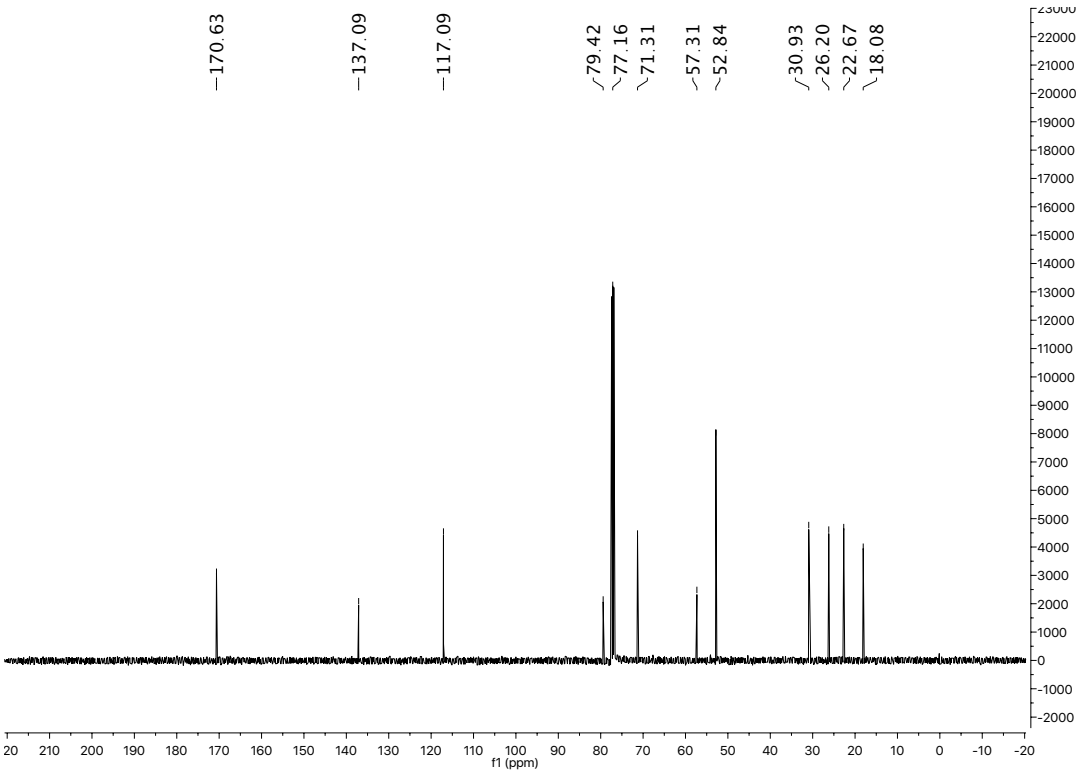




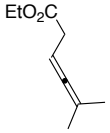
Dimethyl 2-(3-methylbut-2-en-1-yl)-2-(prop-2-yn-1-yl)malonate (9)

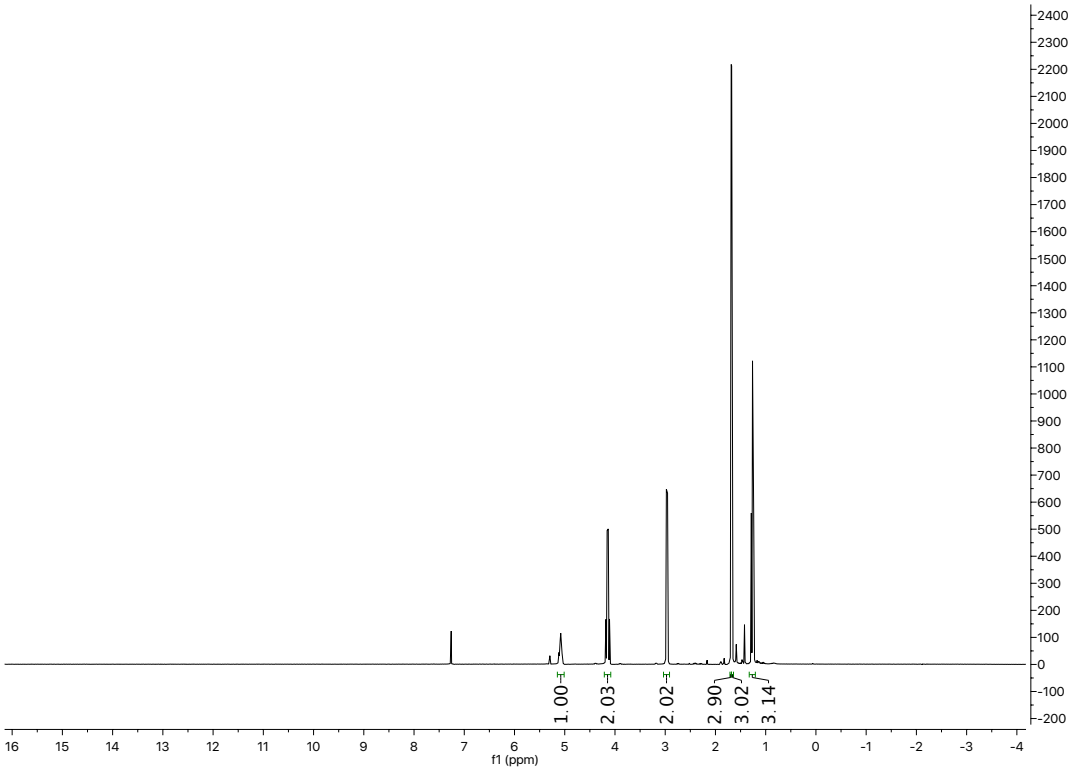


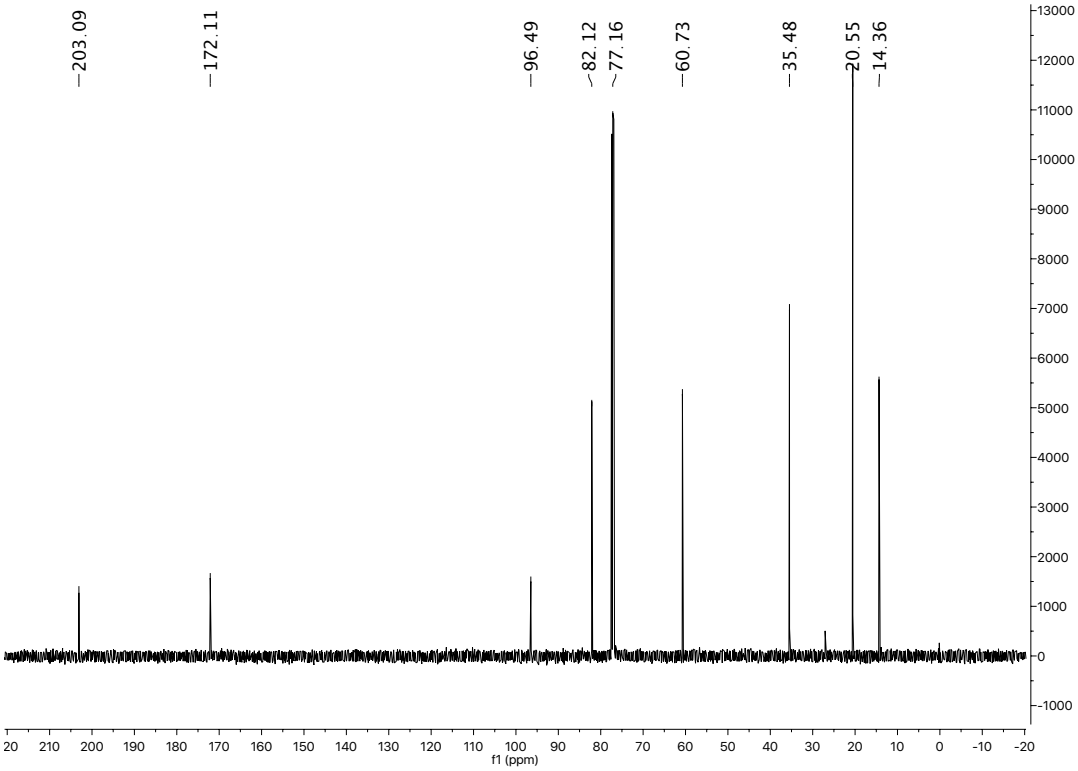




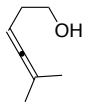
Ethyl 5-methylhexa-3,4-dienoate

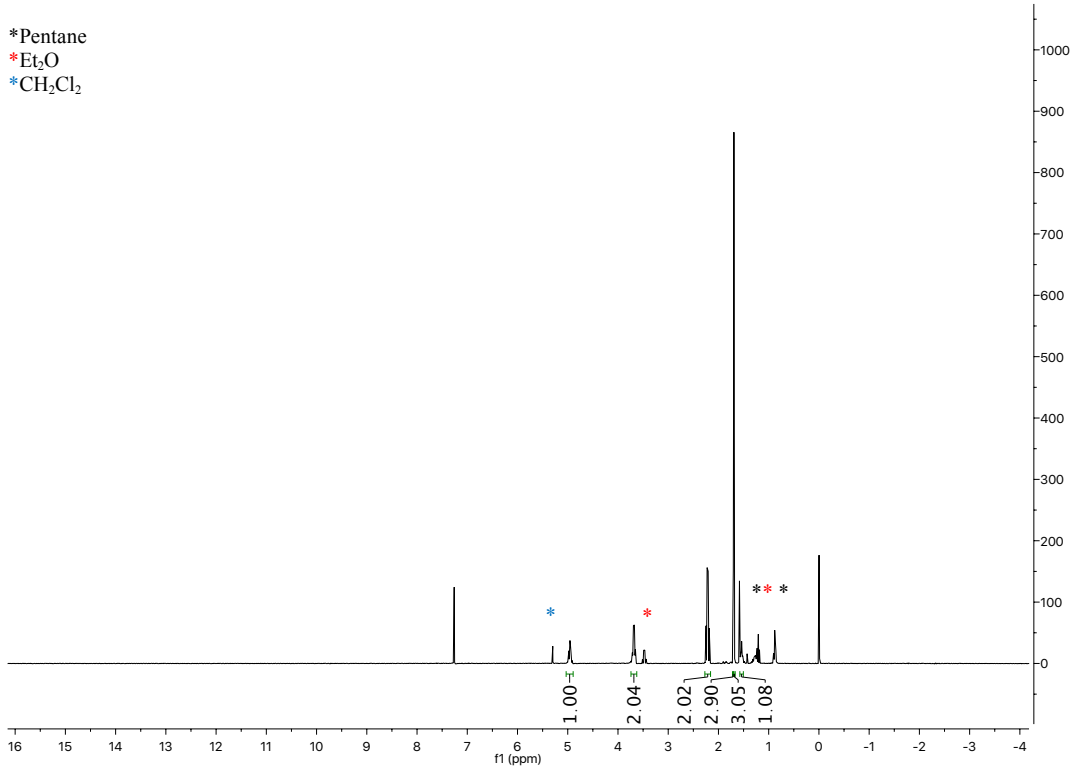


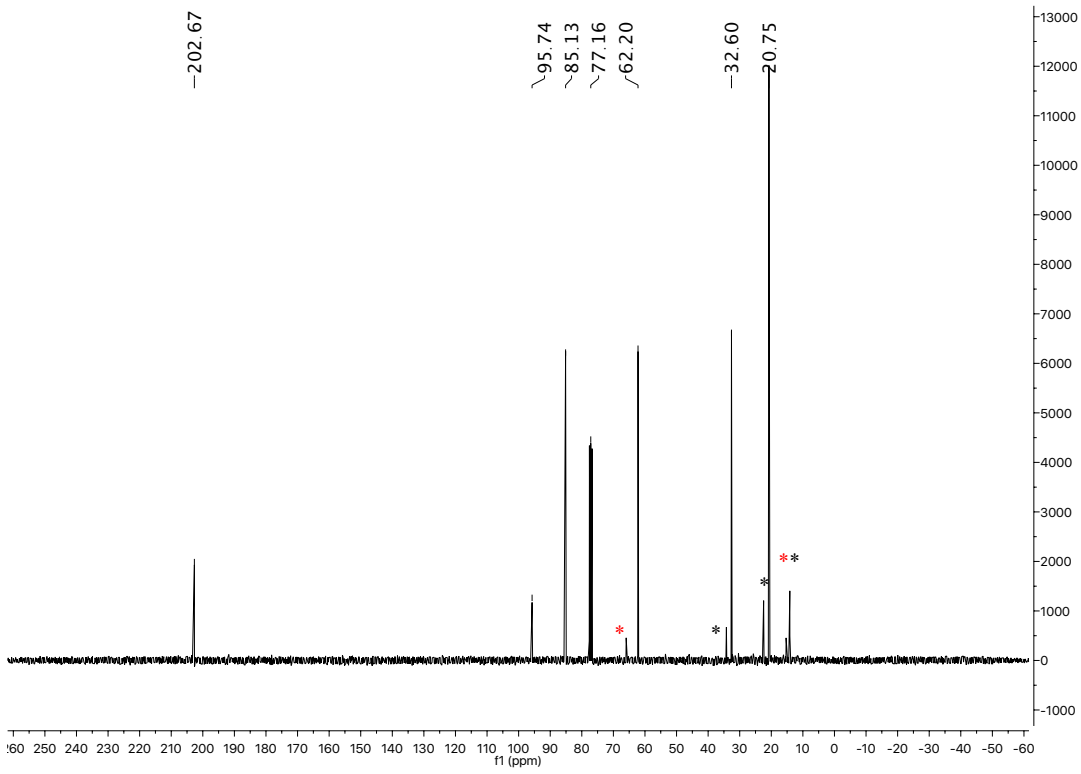




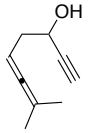
5-methylhexa-3,4-dien-1-ol

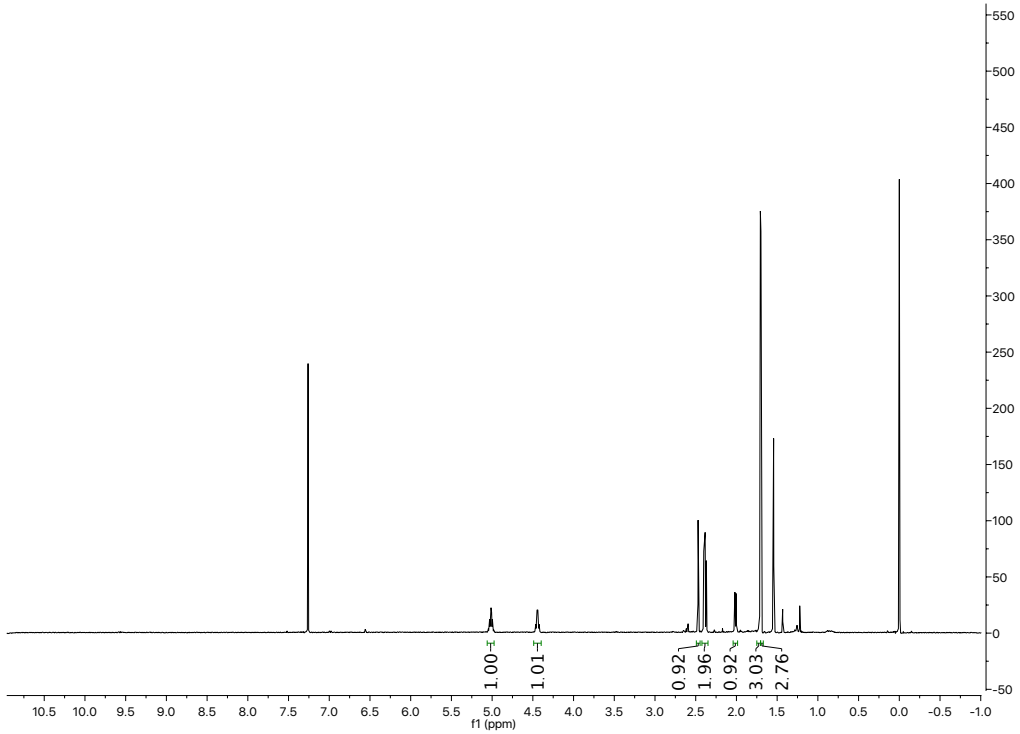


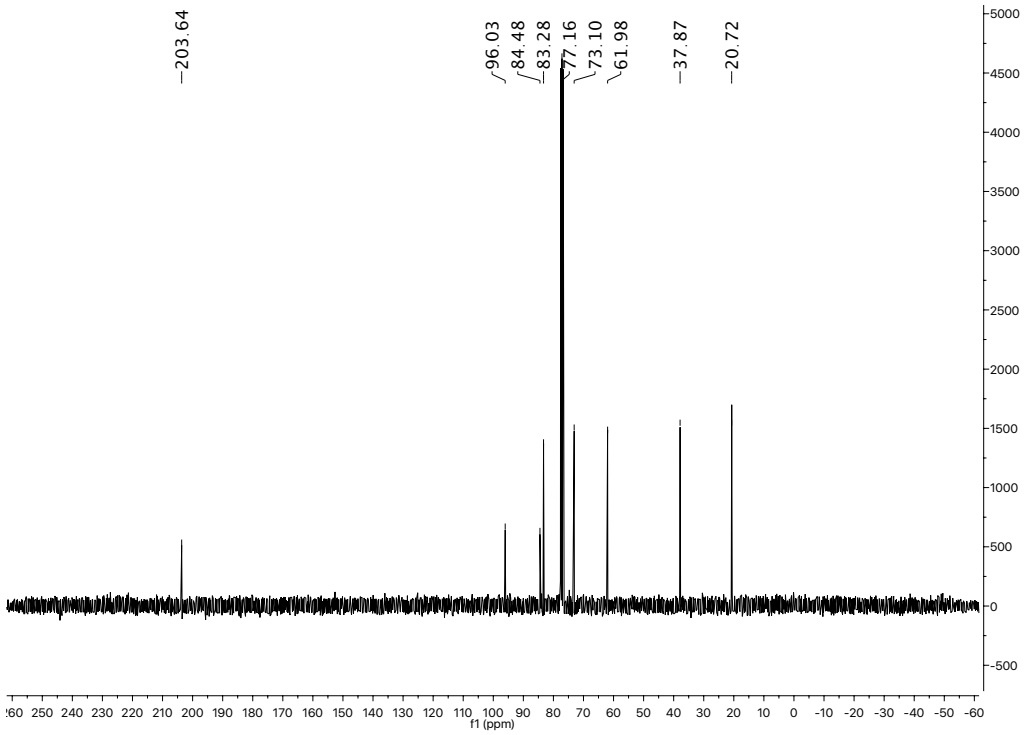




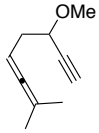
7-methoxylocta-5,6-dien-1-yn-3-ol

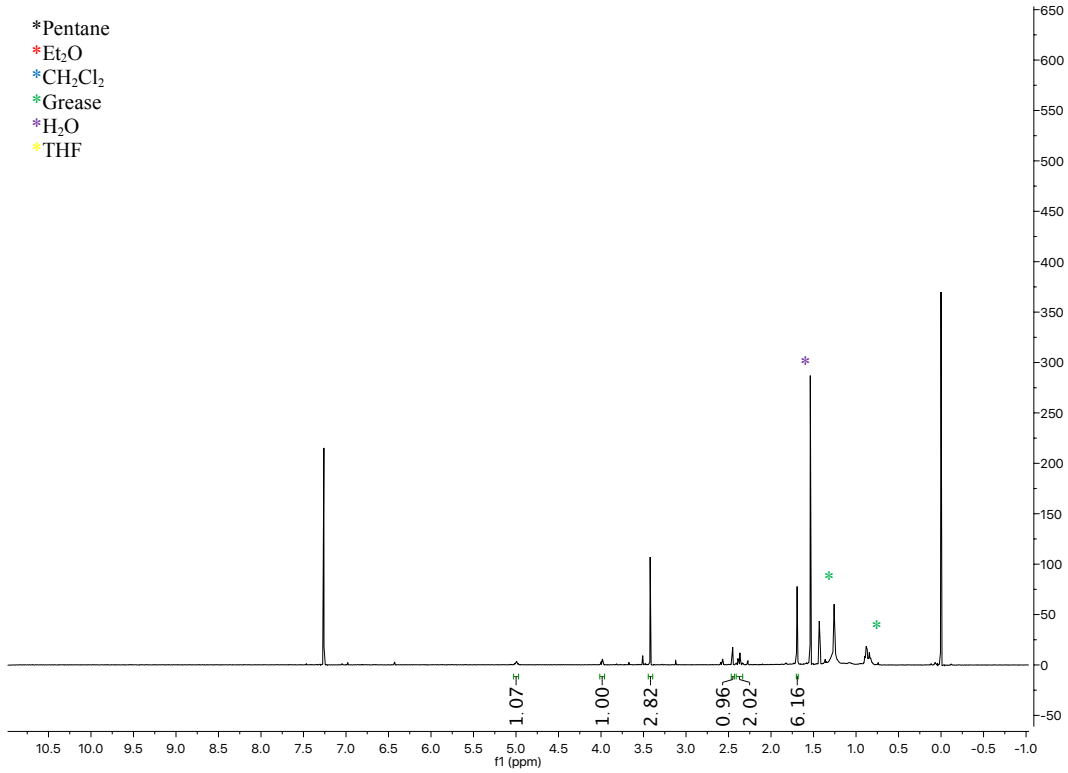


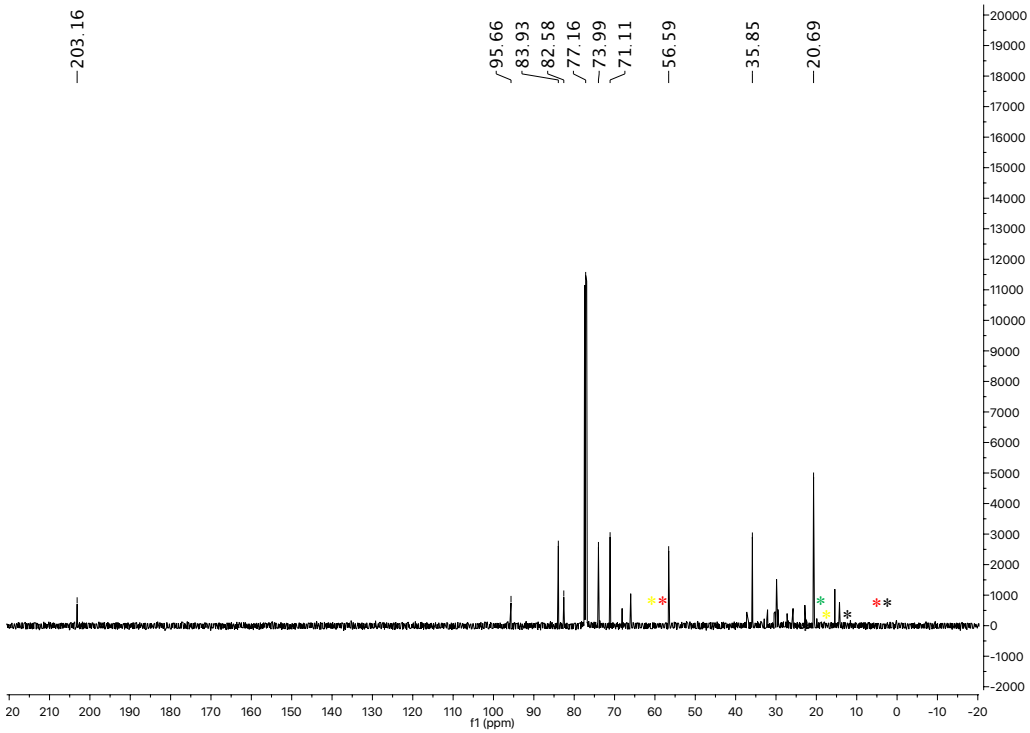




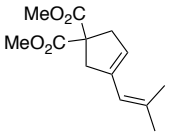
3-methoxy-7-methylocta-5,6-dien-1-yne

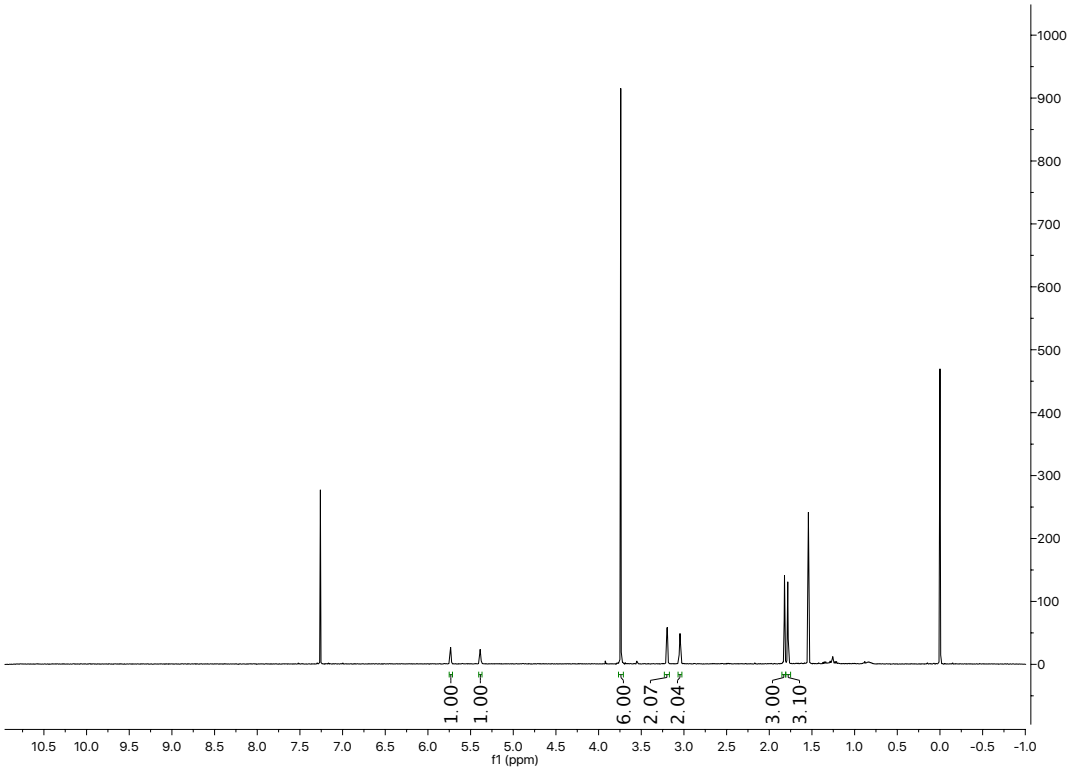


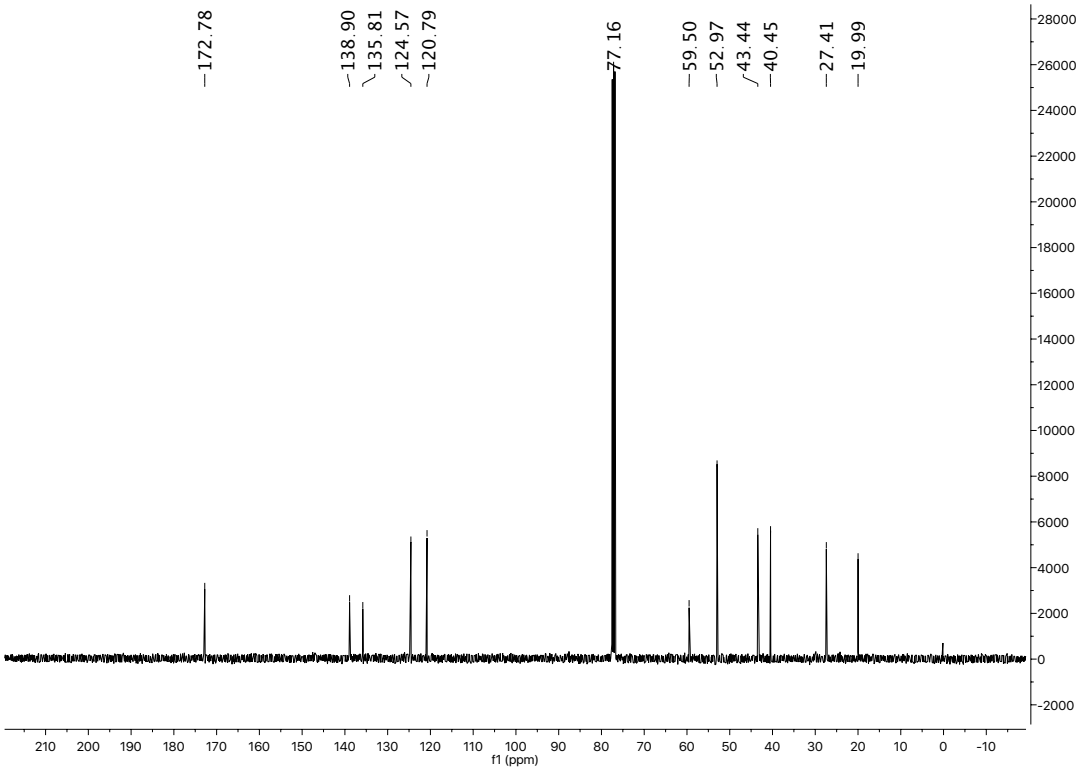




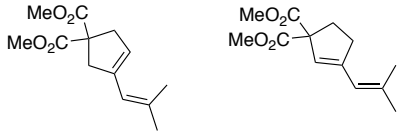
Dimethyl 3-(2-methylprop-1-en-1-yl)cyclopet-3-ene-1,1-dicarboxylate (10a)

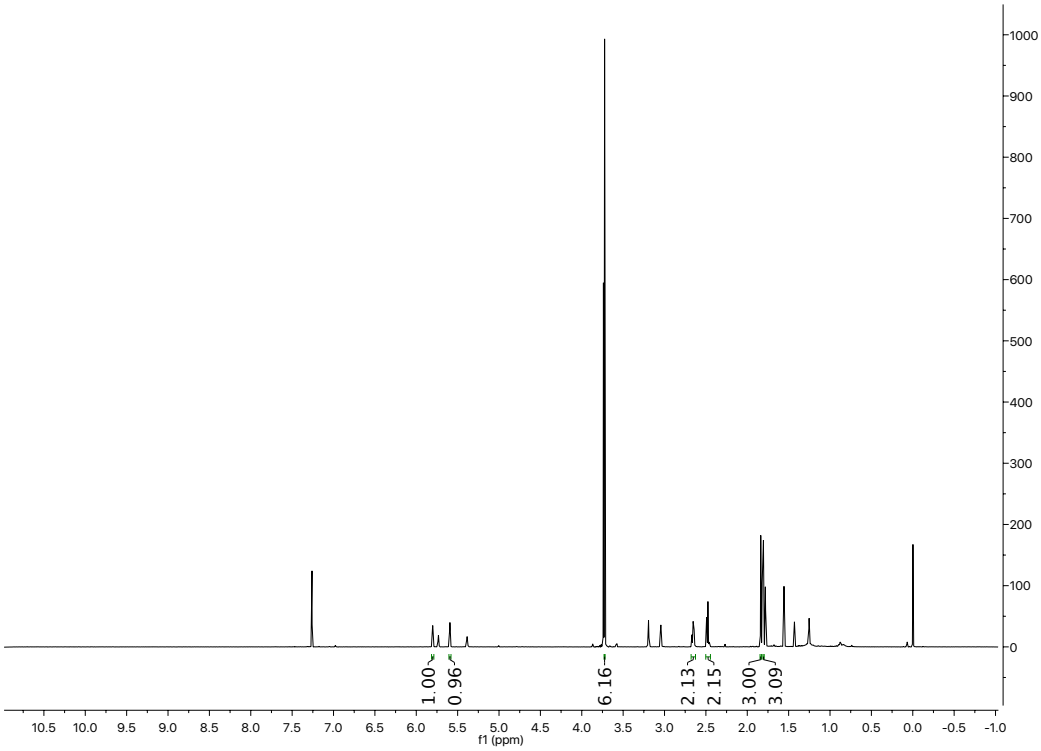


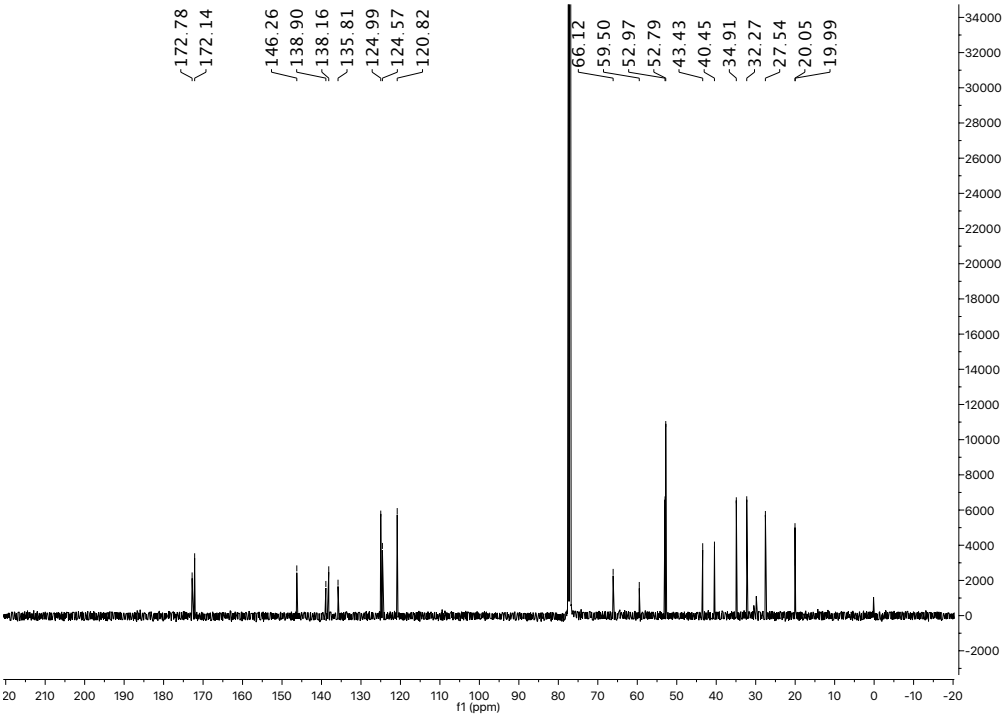




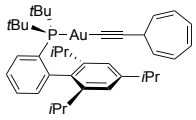
Dimethyl 3-(2-methylprop-1-en-1-yl)cyclopet-3-ene-1,1-dicarboxylate (10a) + Dimethyl 5-(propan-2-ylidene)cyclohex-3-ene-1,1-dicarboxylate (10b) (10a:10b, 1:1.6)

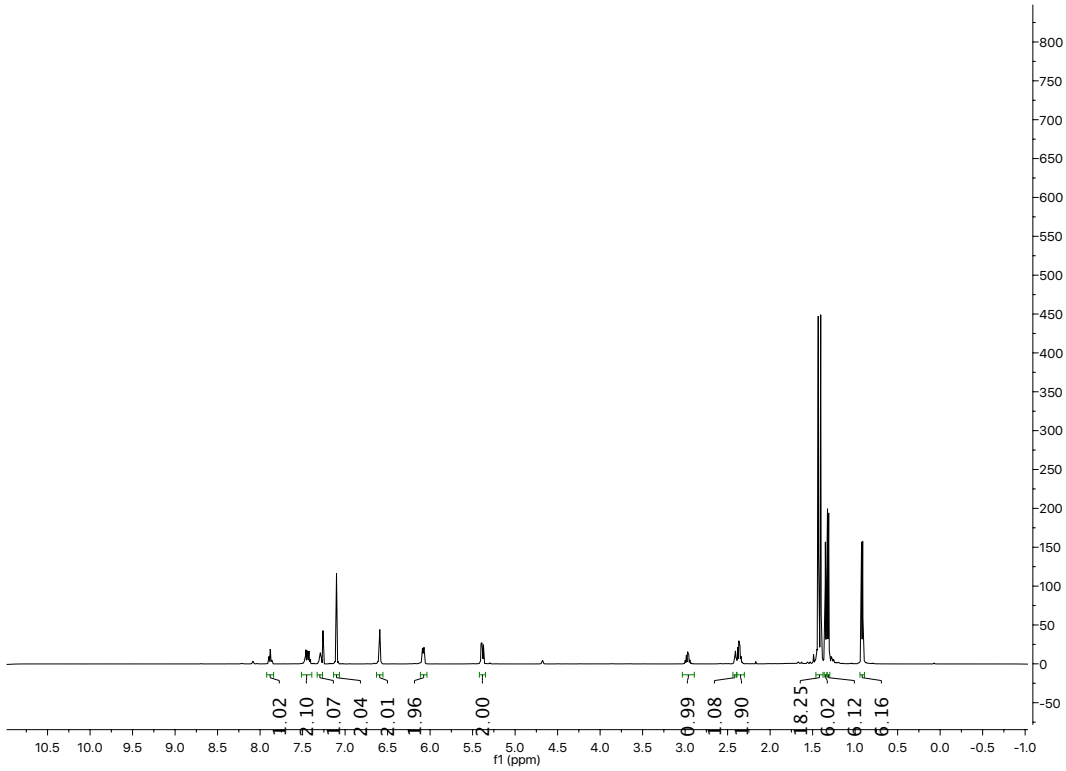


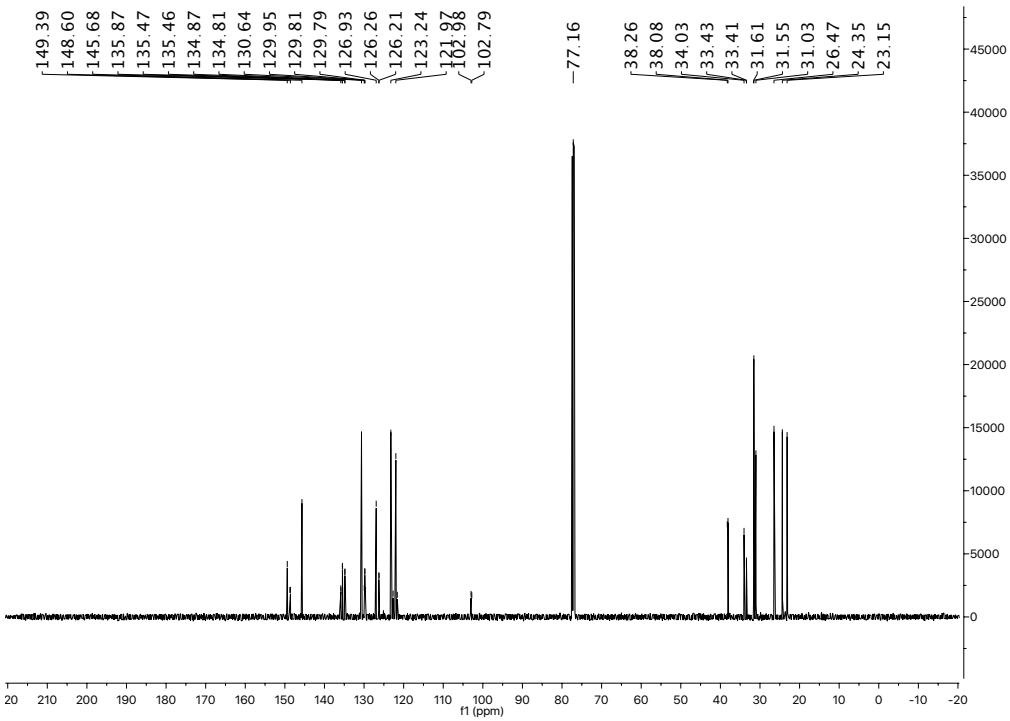


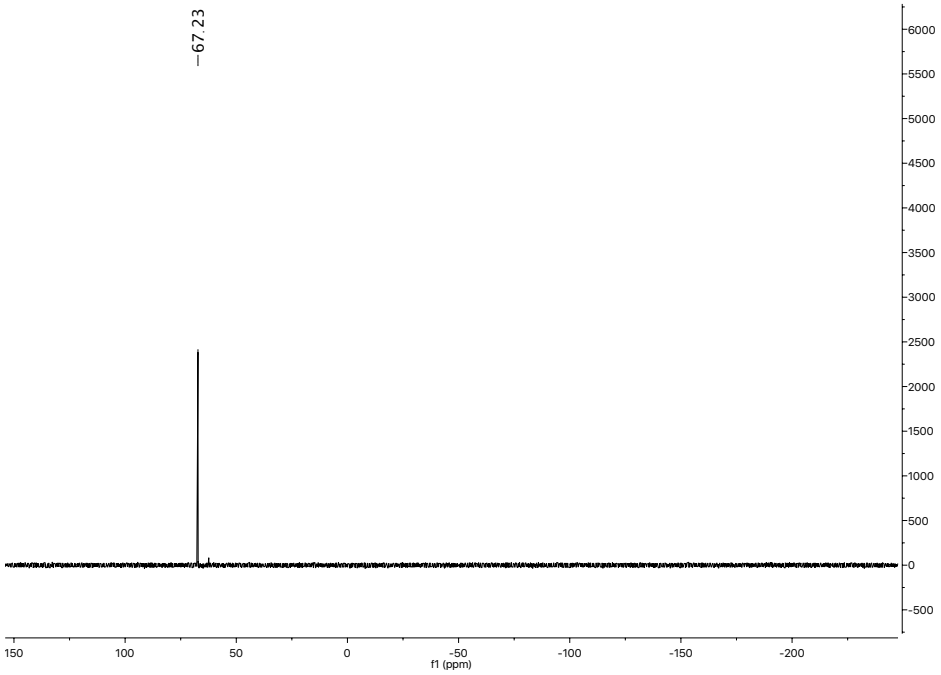


[(2´,4´,6´-Triisopropyl-1,1´-biphenyl-2-yl)di-*tert*-butylphosphine](2- cyclohepta-2,4,6-trien-1-ylethynyl)gold (15)

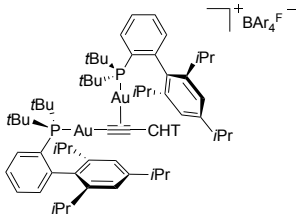


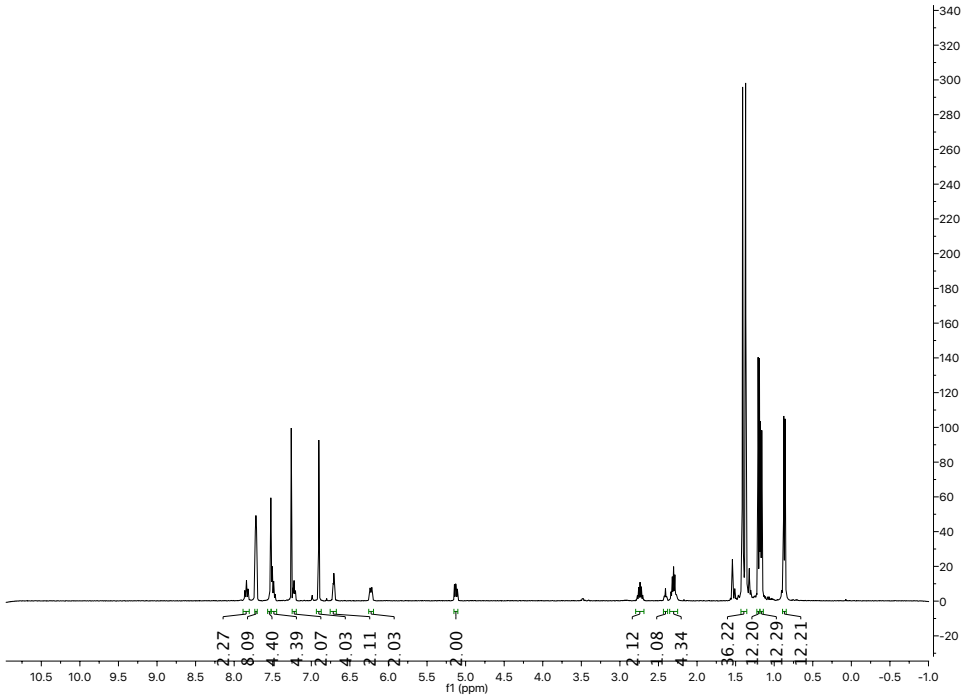


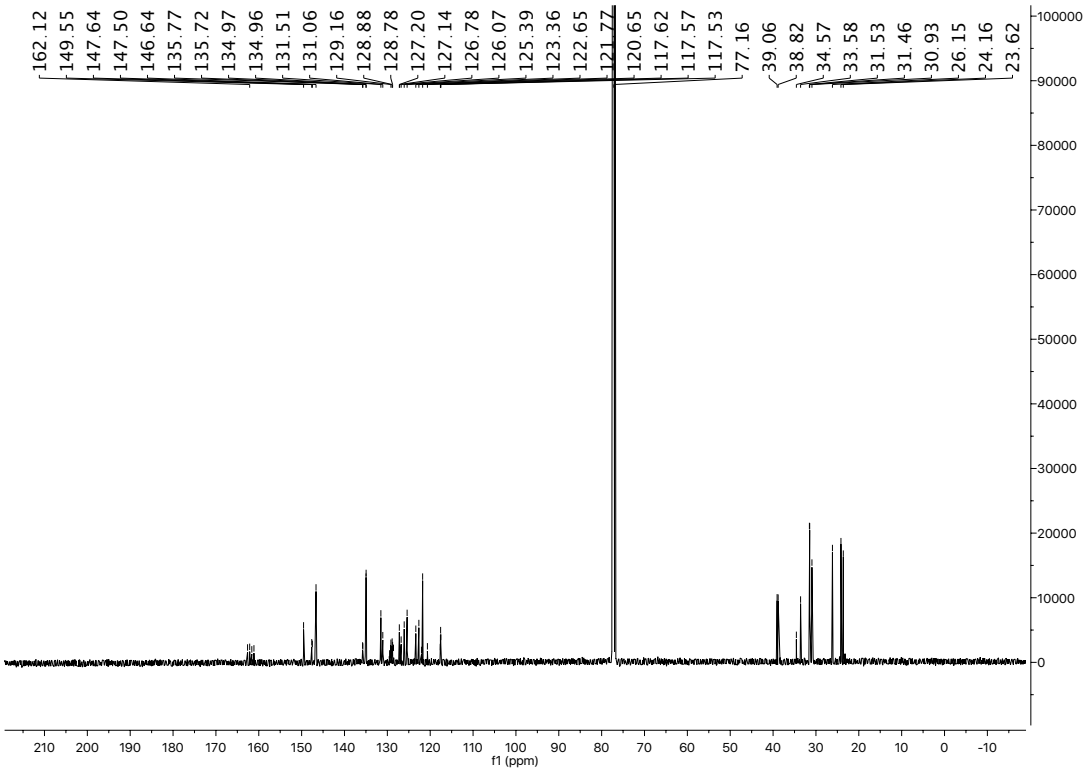


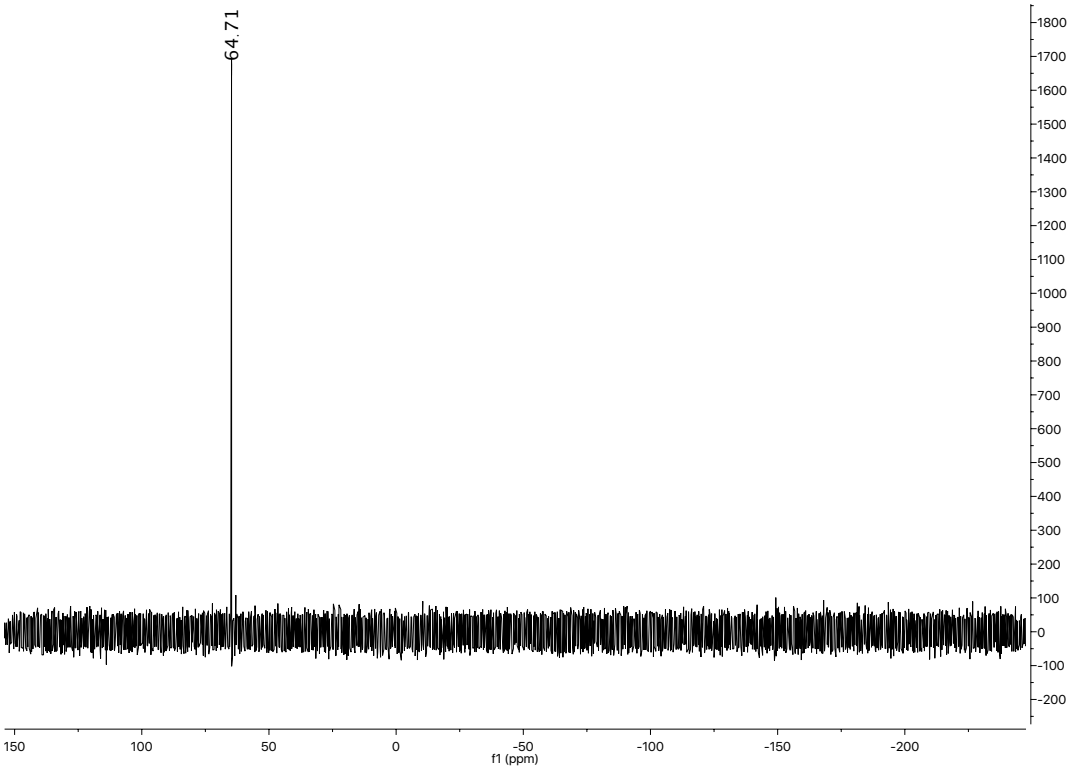


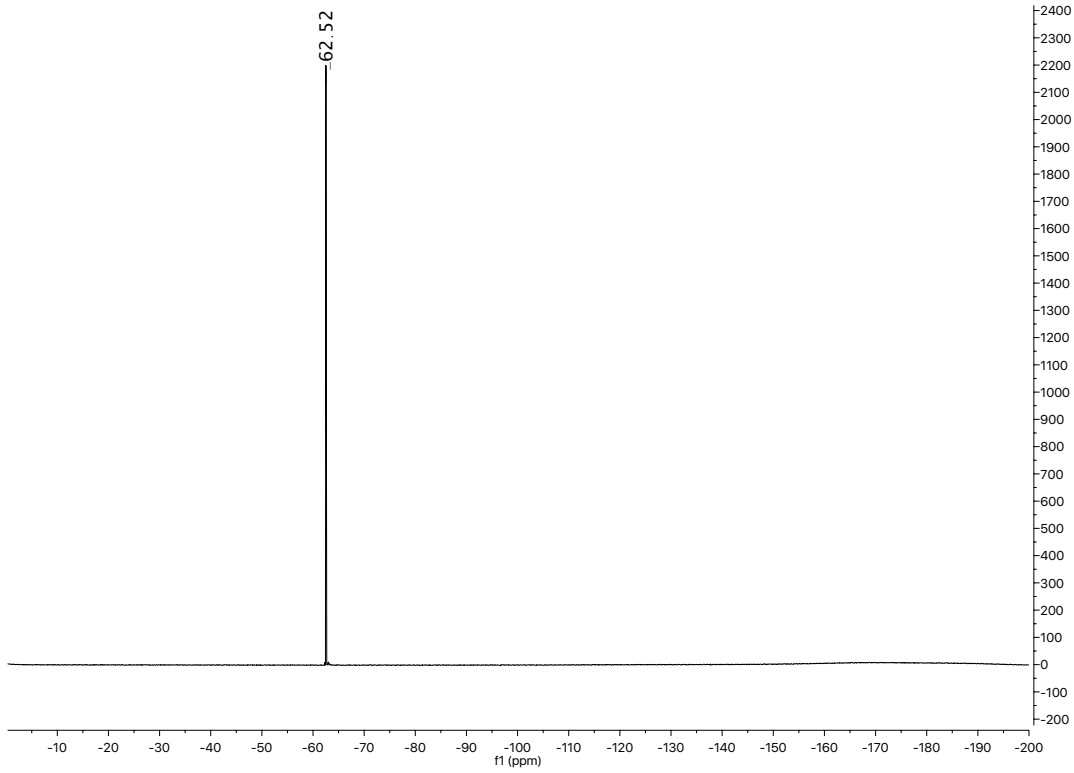
{[(2´,4´,6´-Triisopropyl-1,1´-biphenyl-2-yl)di-*tert*-butylphosphine](2- cyclohepta-2,4,6-trien-1-ylethynyl)gold}[(2´,4´,6´-Triisopropyl-1,1´-biphenyl-2-yl)di-*tert*-butylphosphine] gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (16)

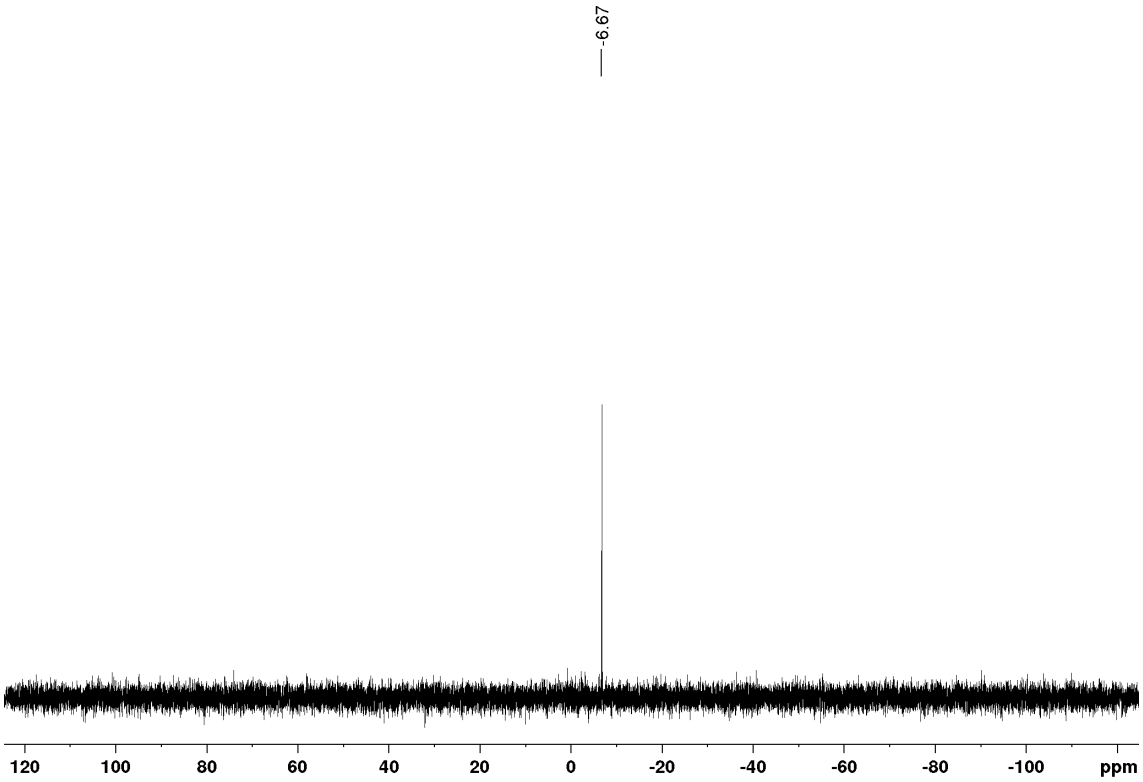




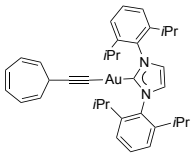

162.12
149.55
147.64
147.50
146.64
135.77
135.72
134.97
134.96
131.51
131.06
129.16
128.88
128.78
127.20
127.14
126.78
126.07
125.39
123.36
122.65
121.77
120.65
117.62
117.57
117.53
77.16
39.06
38.82
34.57
33.58
31.53
31.46
30.93
26.15
24.16
23.62
f1 (ppm)

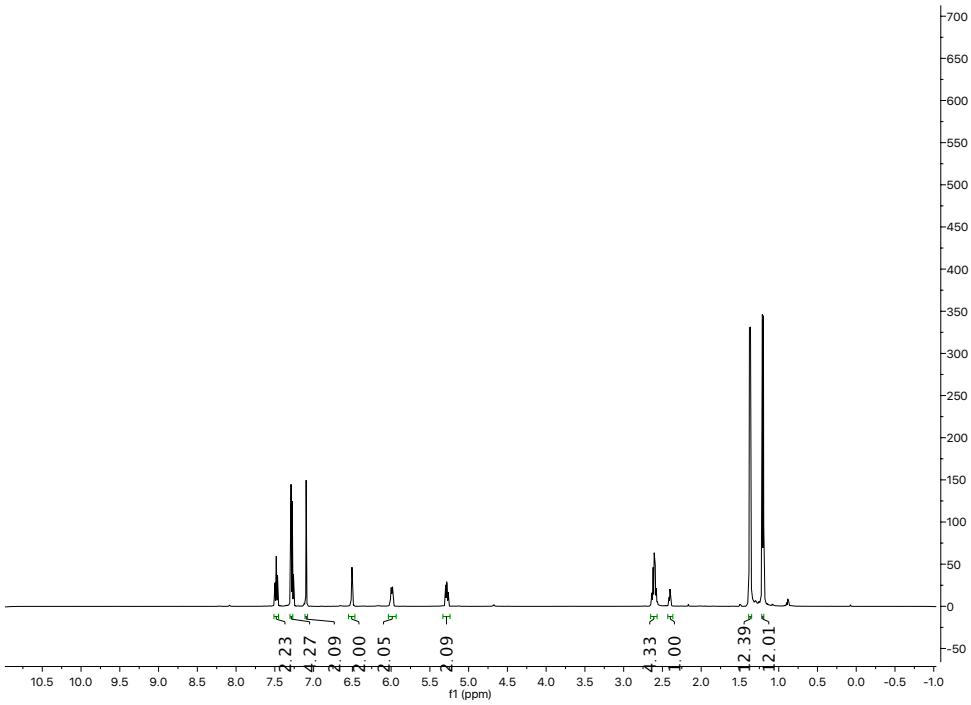

64.71
f1 (ppm)

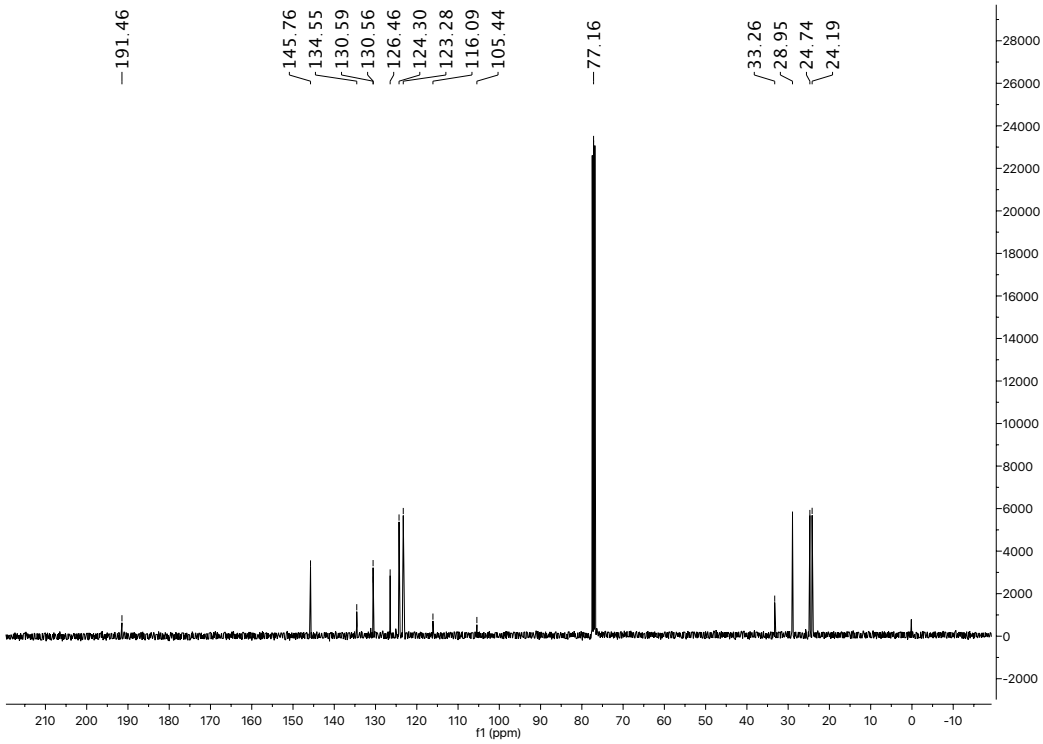

-62.52
f1 (ppm)


-6.67
ppm

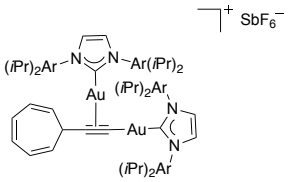
[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl]gold (17)

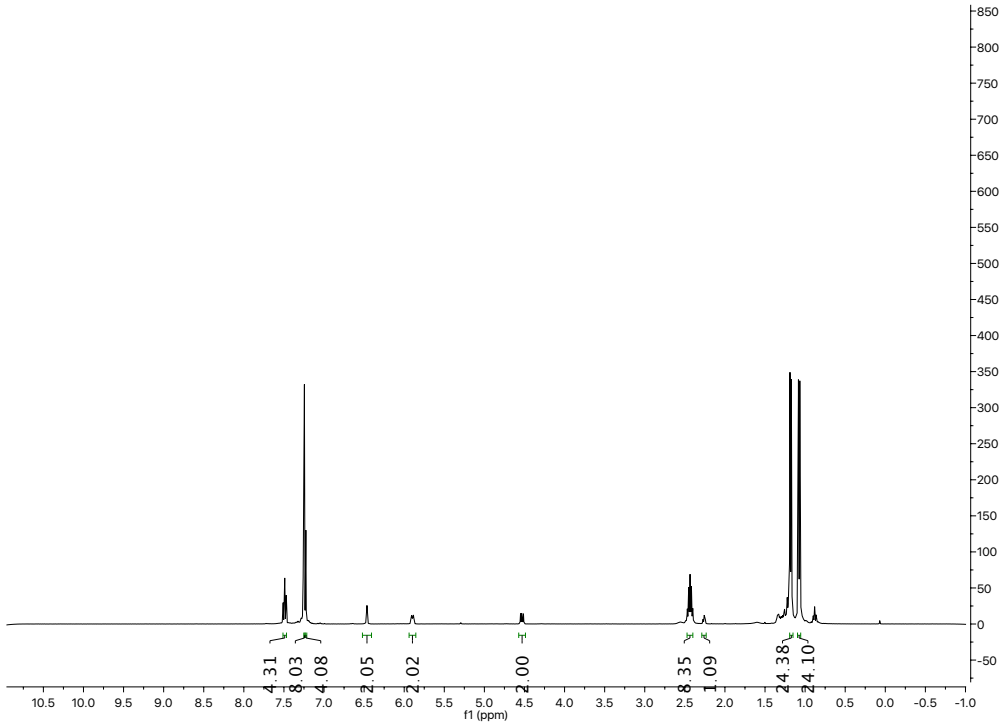


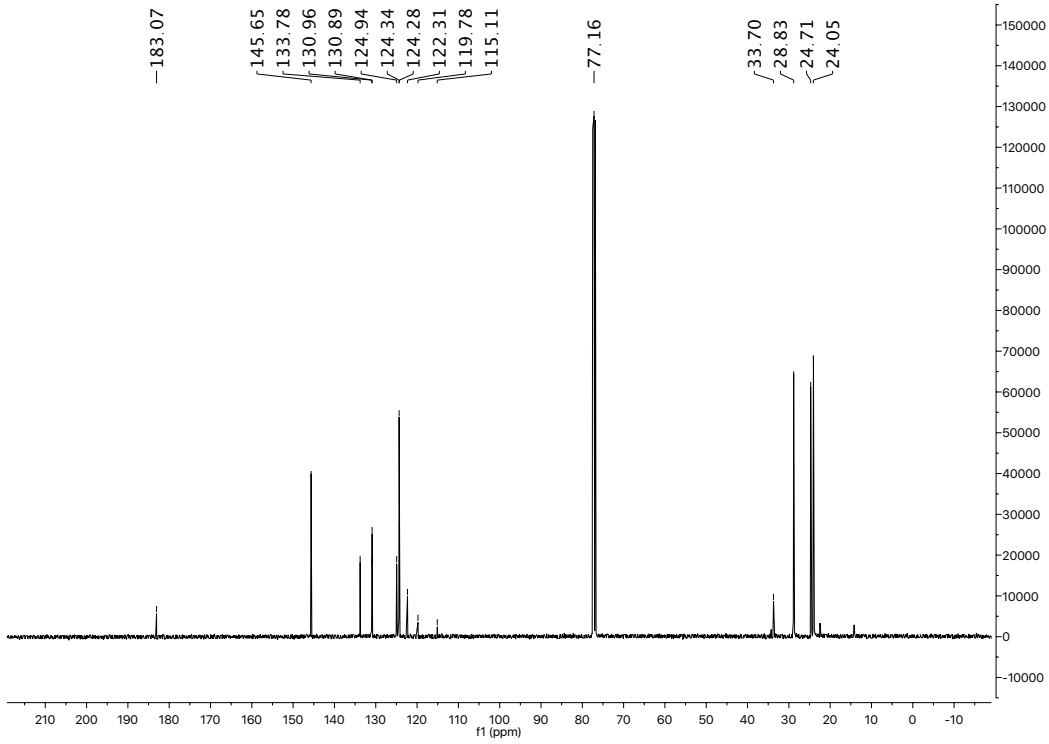




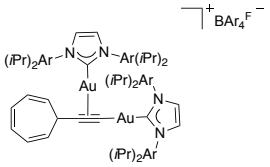
{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (18a)

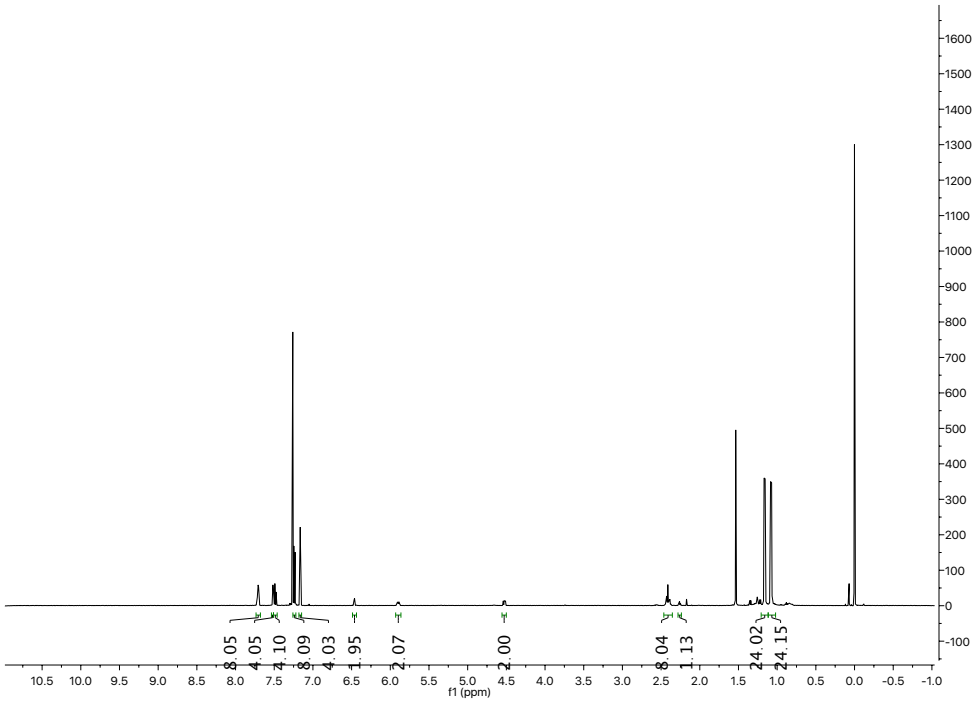


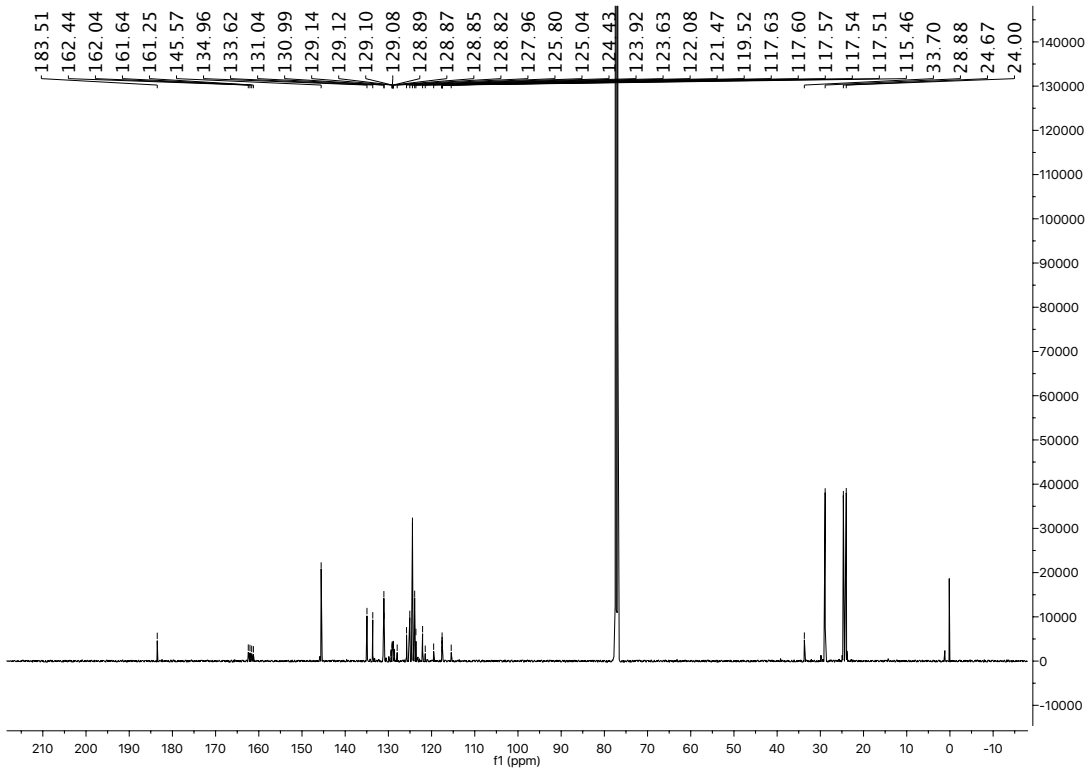


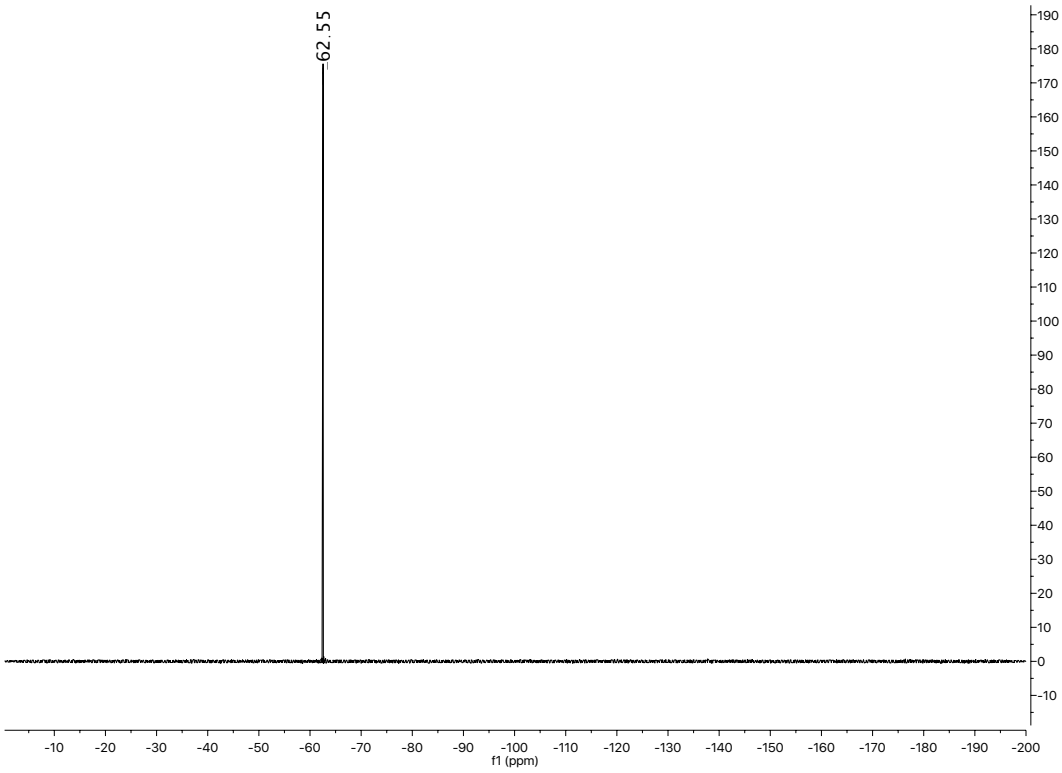


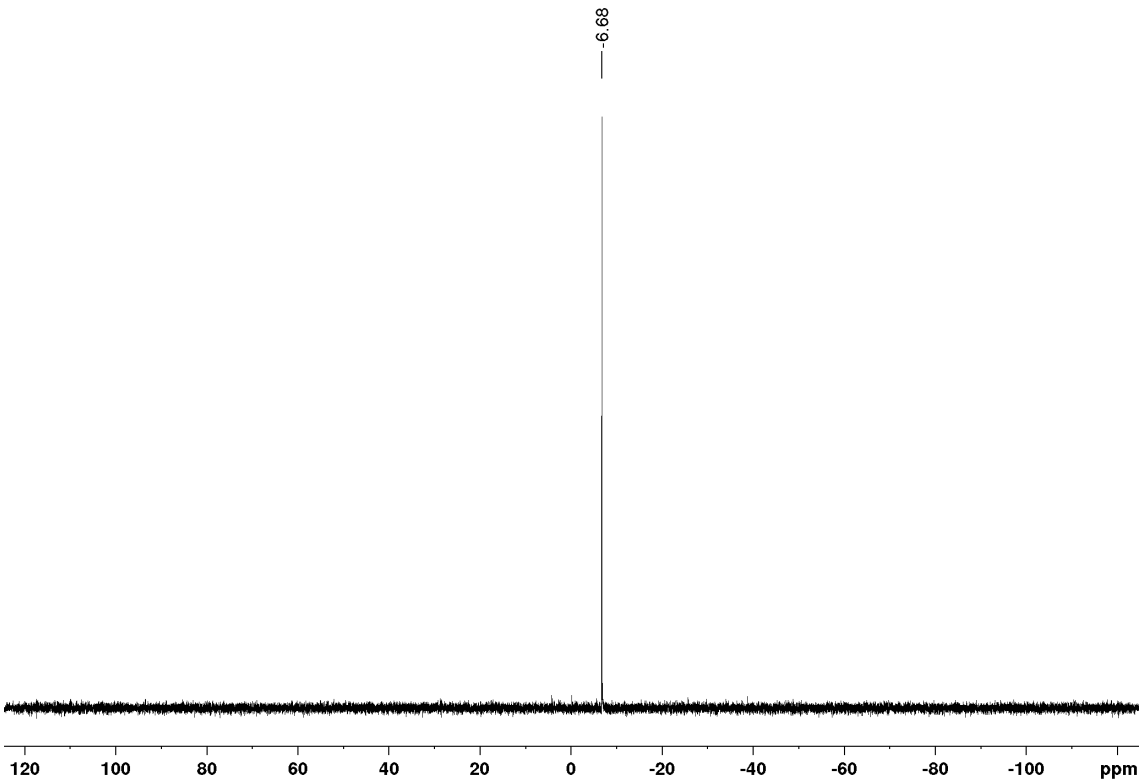
{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)cyclohepta-2,4,6-trien-1-ylethynyl)gold}(1,3-bis(2,6-diisopropylphenyl imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (18b)



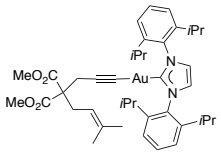


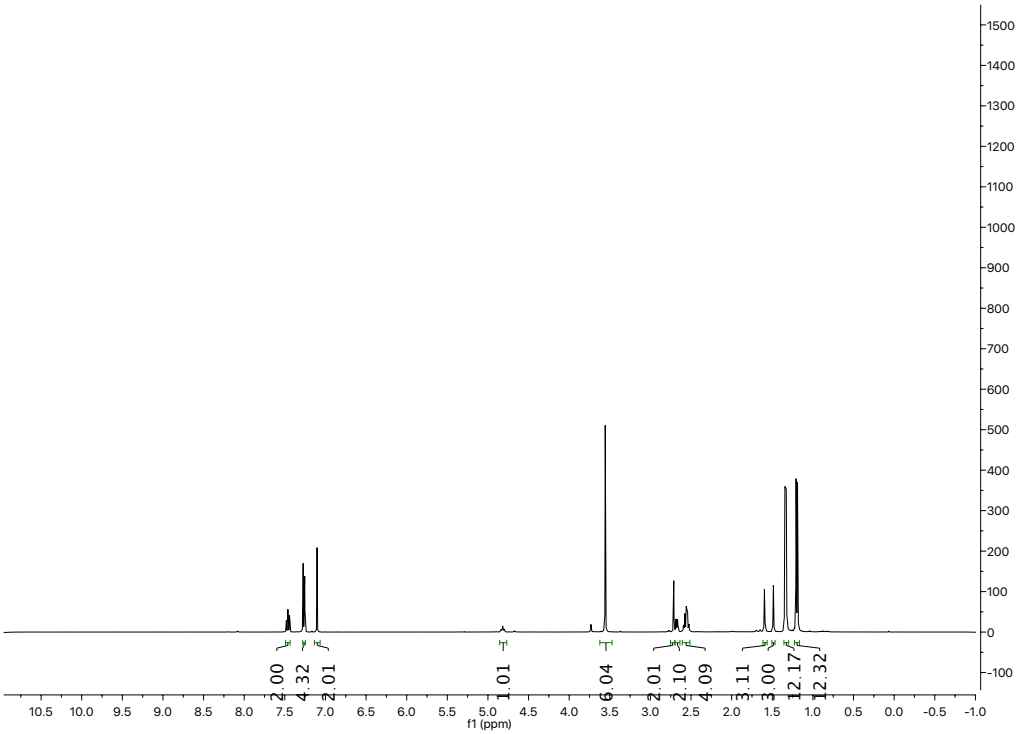


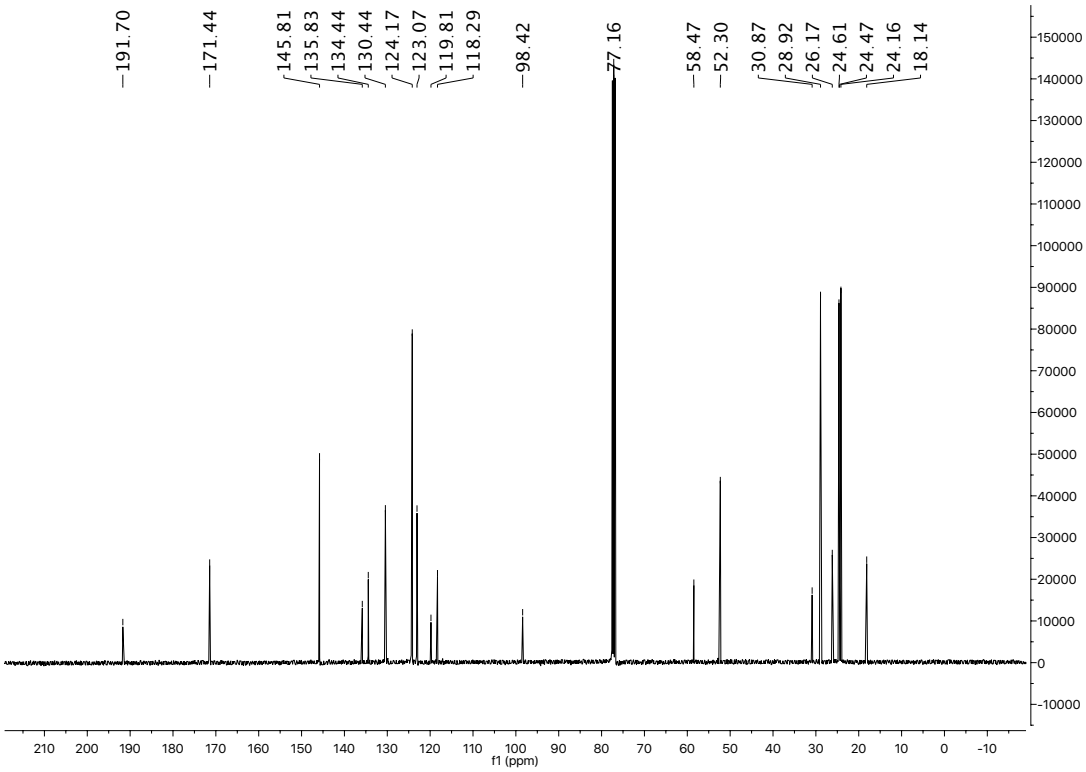

62.55
f1 (ppm)


-6.68
ppm

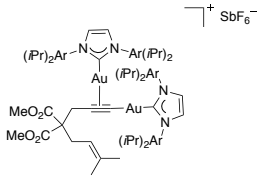
[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)]gold (13)

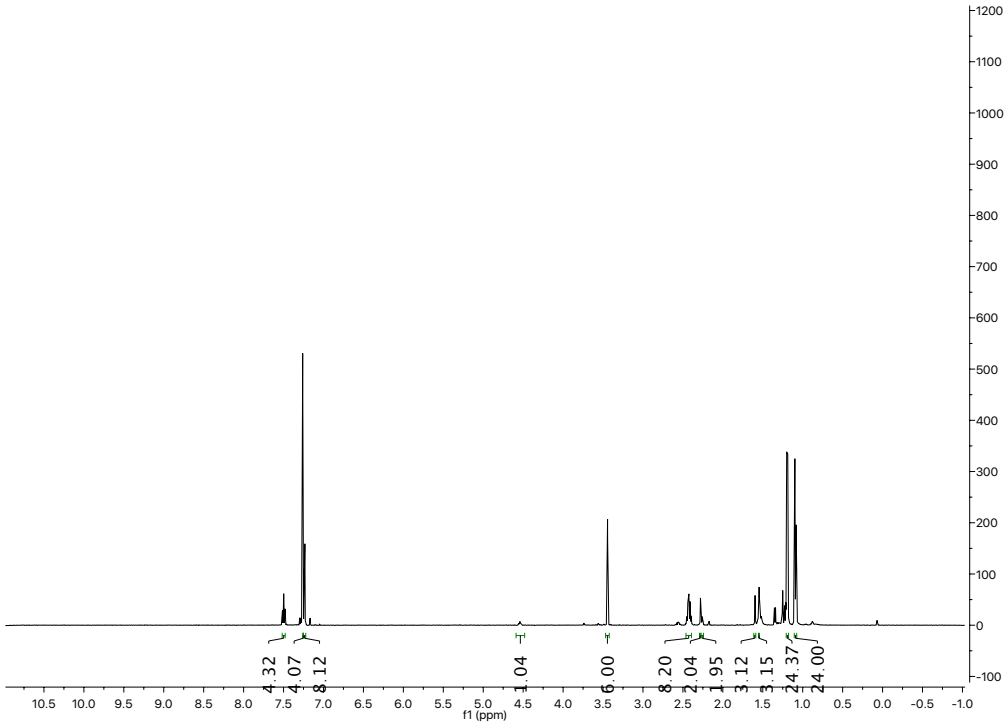


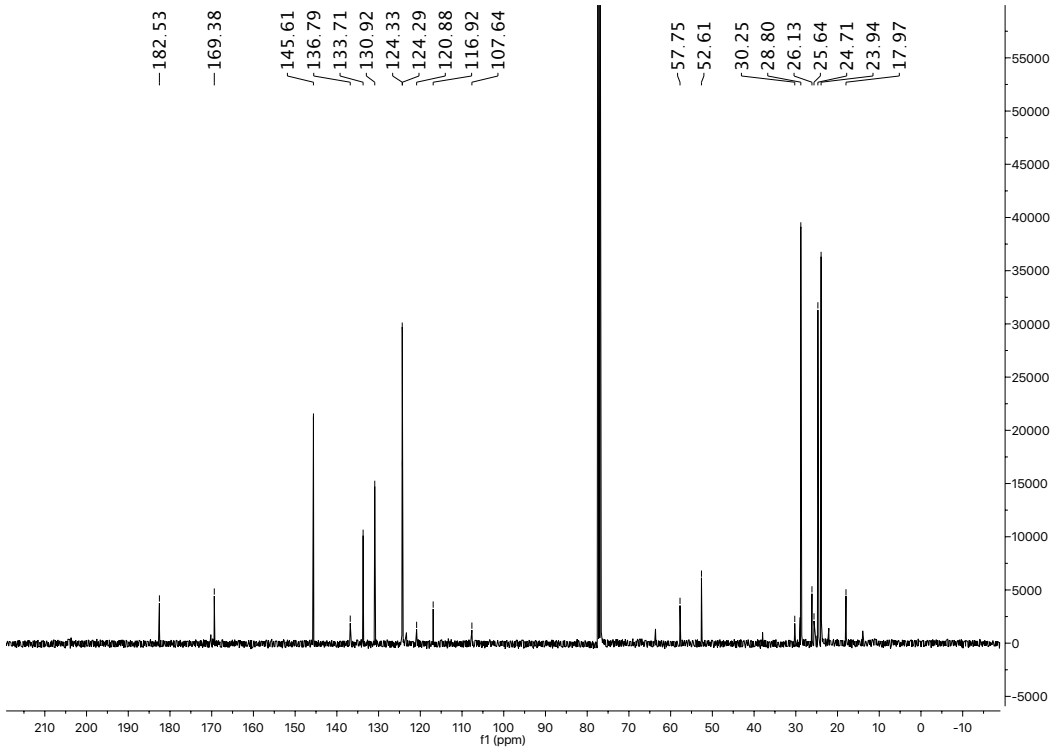




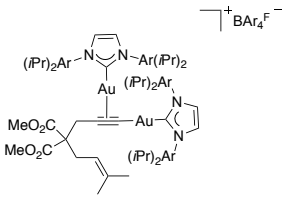
{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold hexafluoroantimonate (14a)

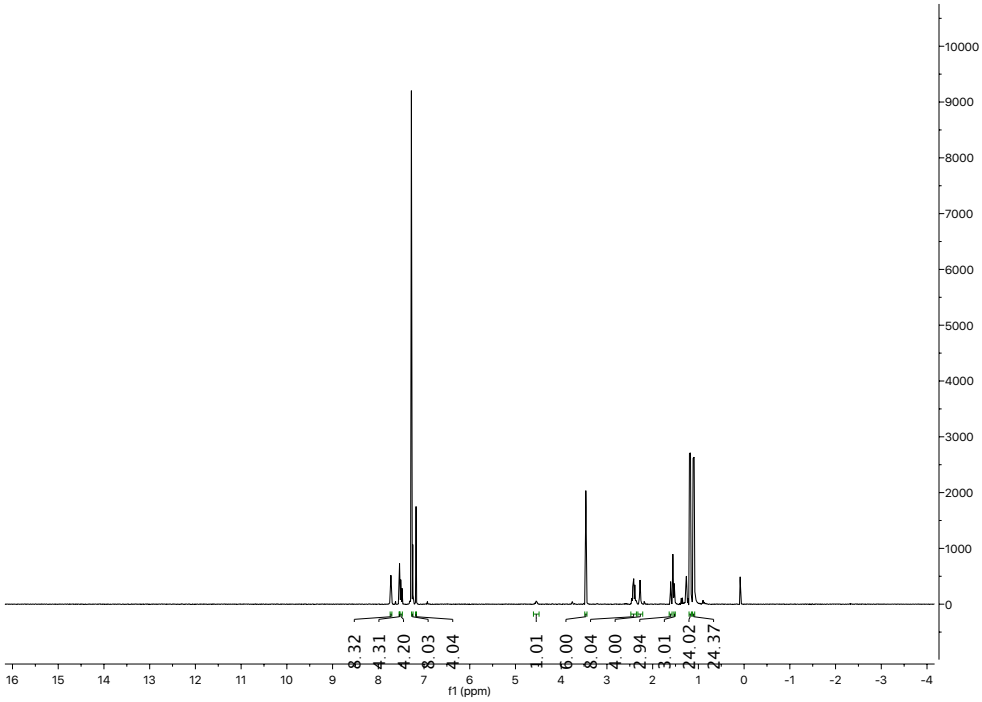


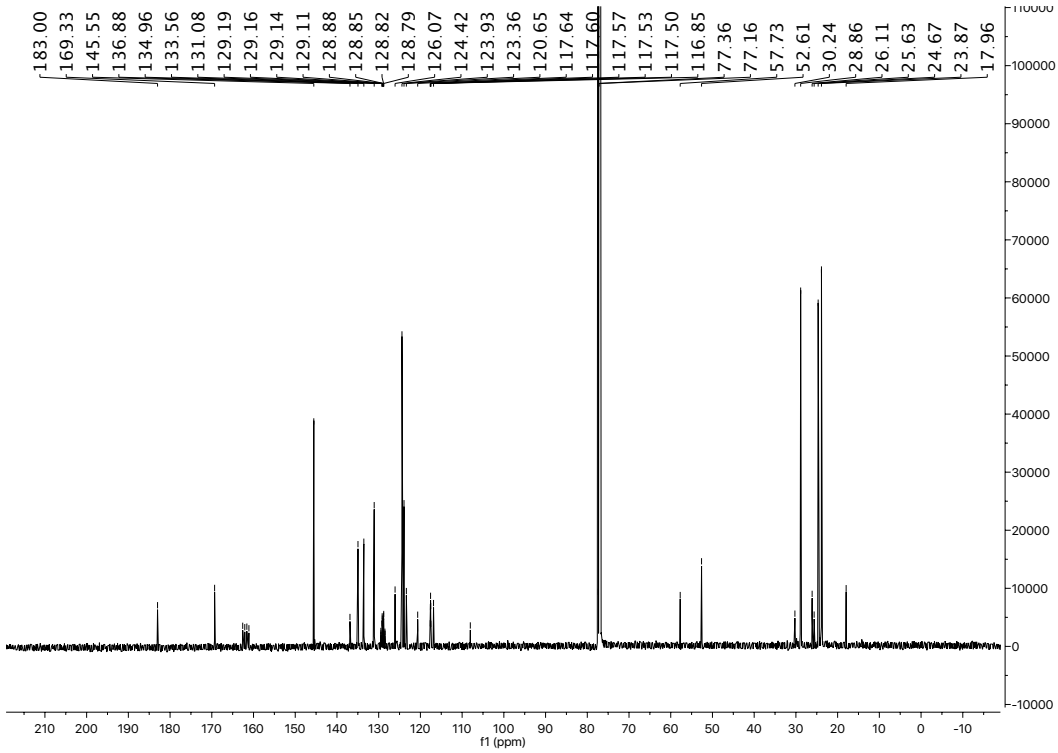


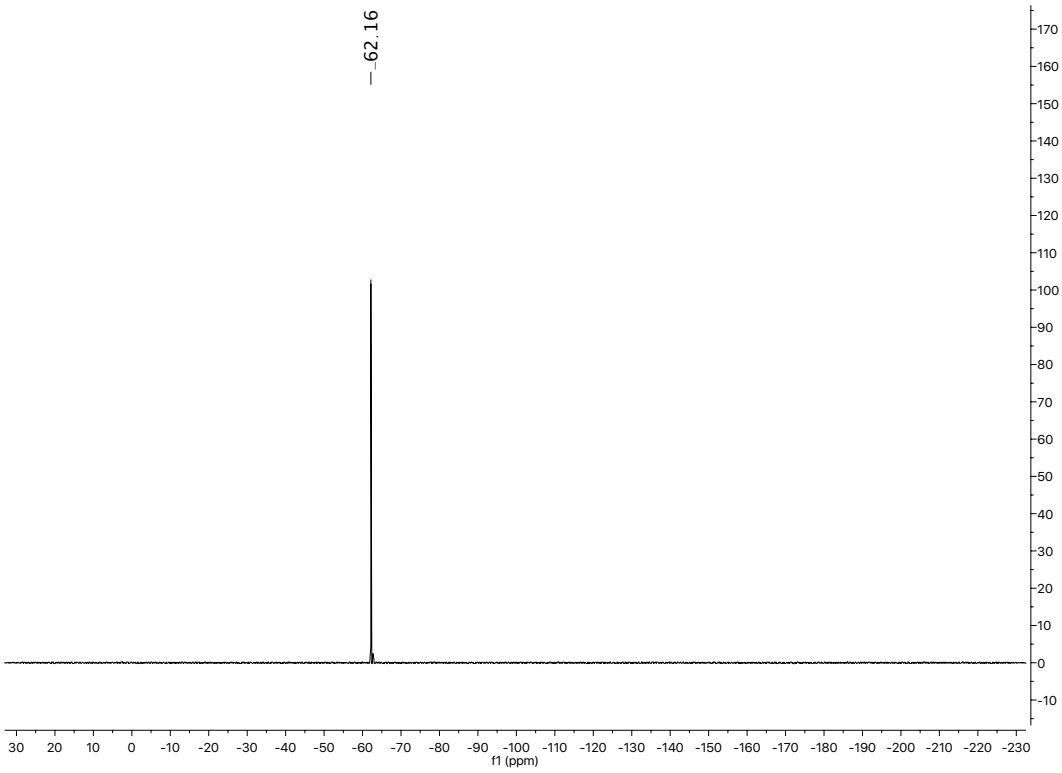


{(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(4,4-bis(methoxycarbonyl)-7-methyloct-6-en-1-yn-1-yl)gold}(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)gold tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (14b)





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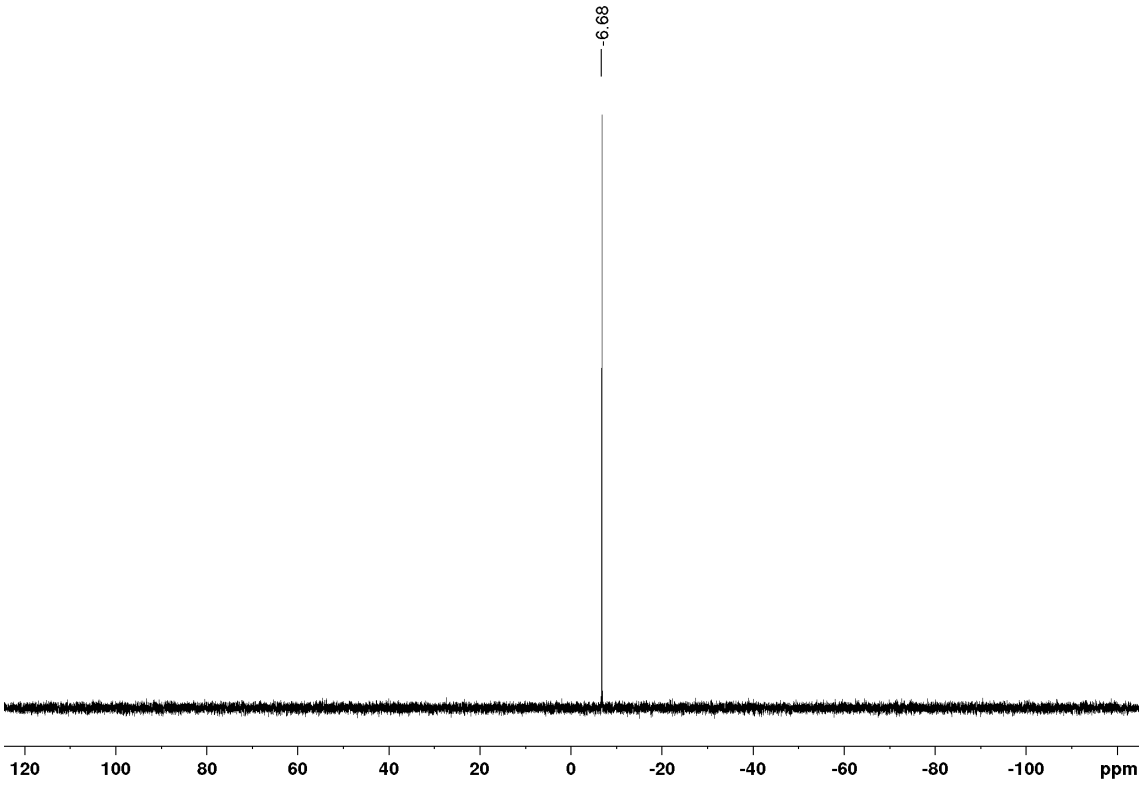
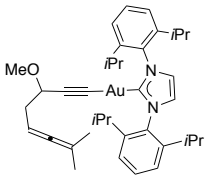
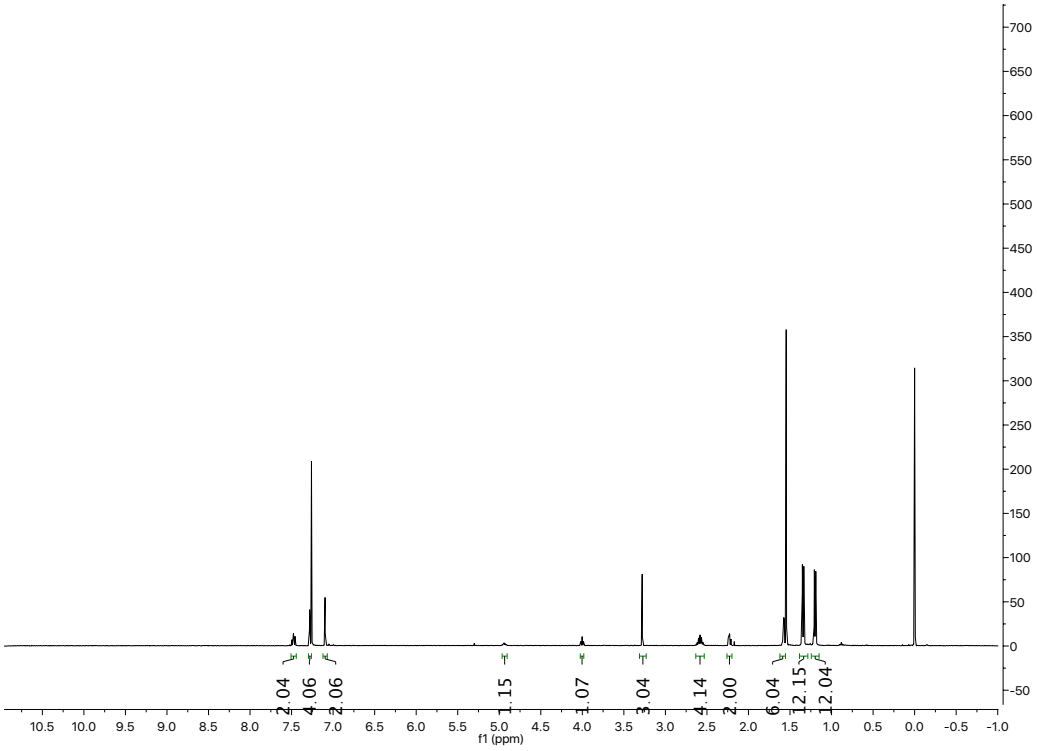
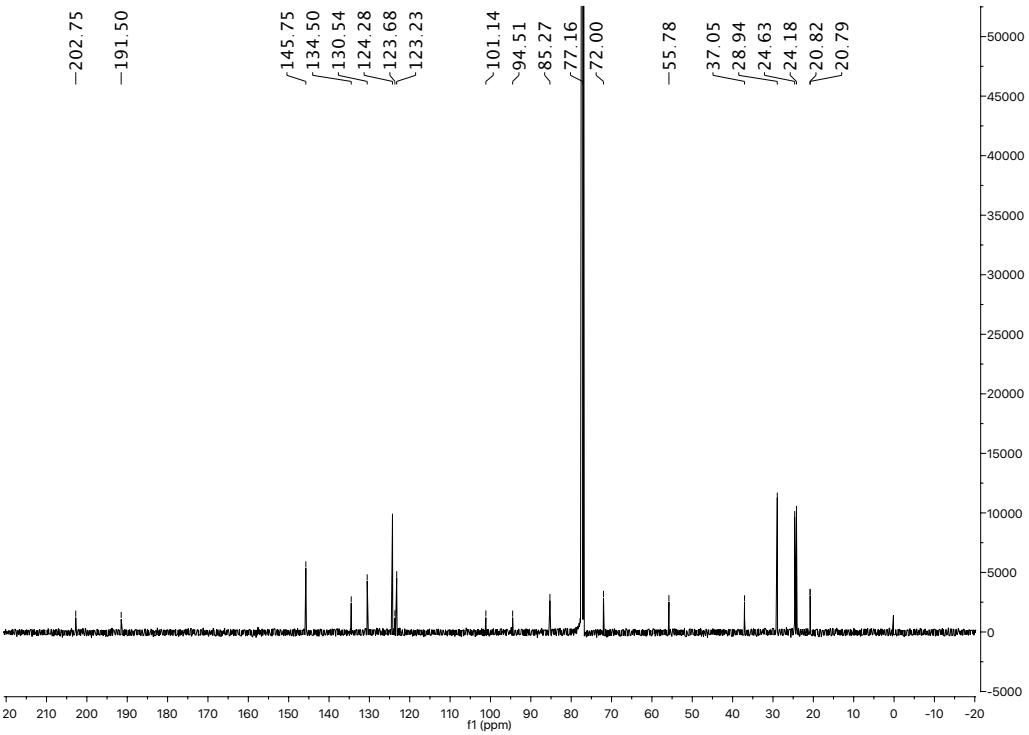
f1 (ppm)


-6.68
ppm

[(1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene)(3-methoxy-7-methylocta-5,6-dien-1-yne)]gold (19)







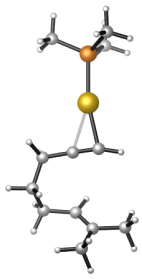
6. Theoretical DFT Computations

6.1. Computational Methods

Calculations were performed by means of the Gaussian 09 suite of programs.[4] DFT was applied using **M06**[5] and **B3LYP**[6]. The SDD basis set and ECP was used to describe Au.[7] The 6-31G(d) basis set[8] was used for all remaining atoms (C, H, N and P). Full geometry optimizations were carried out in dichloromethane, through an implicit solvent SMD[9]. The stationary points were characterized by vibrational analysis. Transition states were identified by the presence of one imaginary frequency while minima by a full set of real frequencies. The connectivity of the transition states was confirmed by relaxing each transition state towards both the reactant and the product. Reported energies are potential energies (E) and free energies (G) in solution, computed at 298 K and 1 atm.

6.2 Coordinates and Energies of Relevant Intermediates and Transition States (M06, L_1 = PMe_3, a series; L_2 = PPh_3, b series; L_3 = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene), c series)

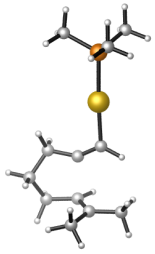
Ia



E = -947.658518 h.
G = -947.339946 h.

6	0.731633	0.029111	0.939980
1	-0.344880	0.021561	0.984544
6	1.926109	-0.102656	1.208517
6	3.328900	-0.314325	1.553067
1	3.823982	-0.782527	0.690510
1	3.814268	0.662610	1.704110
6	3.223683	-0.482637	4.118243
1	3.470843	-1.171948	4.938686
1	3.909520	0.372348	4.218682
6	1.805288	-0.005928	4.228172
1	1.615078	1.021466	3.902254
6	0.749684	-0.732187	4.623290
6	0.831177	-2.157502	5.075101
1	0.352383	-2.284115	6.058089
1	0.282261	-2.814278	4.382264
1	1.857609	-2.535100	5.148608
6	-0.634278	-0.160709	4.604948
1	-1.290872	-0.748415	3.943330
1	-1.096846	-0.199341	5.603268
1	-0.647135	0.881866	4.261416
79	1.559513	1.024410	-0.888814
15	1.922633	2.120433	-2.912696
6	3.616562	1.925125	-3.544199
1	3.835139	0.862557	-3.701925
1	3.720057	2.461309	-4.497183
1	4.334012	2.330293	-2.820975
6	1.648982	3.915046	-2.829078
1	1.816724	4.364428	-3.817111
1	0.620920	4.122061	-2.509589
1	2.339557	4.362485	-2.104721
6	0.845264	1.537532	-4.255617
1	-0.206538	1.694956	-3.989267
1	1.071638	2.092862	-5.175977
1	1.009501	0.467605	-4.429300
6	3.523268	-1.194874	2.798074
1	2.897496	-2.095308	2.708284
1	4.569434	-1.529308	2.791945

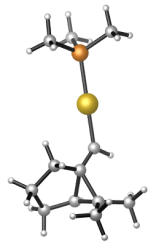
TS_{Ia-IIa}



E = -947.648180 h.
G = -947.378038 h.

6	1.108817	0.887419	1.523645
1	0.125097	1.126651	1.923441
6	2.102744	0.350928	2.133689
6	3.509815	-0.097383	2.050460
1	3.689449	-0.420736	1.015438
1	4.164343	0.766832	2.247155
6	3.374985	-0.697366	4.418894
1	3.324439	-1.521712	5.144022
1	4.115638	0.017707	4.799910
6	2.049350	0.001030	4.292526
1	2.015470	1.067033	4.530100
6	0.845215	-0.639018	4.170764
6	0.696412	-2.110098	3.994108
1	-0.149359	-2.475746	4.591918
1	0.450231	-2.334620	2.944462
1	1.591044	-2.680327	4.264362
6	-0.421125	0.134283	4.191705
1	-1.059697	-0.130694	3.334726
1	-0.994602	-0.139508	5.090464
1	-0.257593	1.217618	4.210505
79	1.453894	1.386065	-0.501342
15	1.697386	1.970469	-2.760972
6	3.294510	1.523413	-3.512935
1	3.449105	0.439832	-3.448204
1	3.307333	1.827113	-4.568545
1	4.111972	2.026538	-2.982817
6	1.531795	3.754175	-3.091517
1	1.625804	3.945024	-4.169144
1	0.554472	4.111041	-2.745392
1	2.314515	4.306355	-2.557837
6	0.458293	1.194861	-3.846857
1	-0.549984	1.491313	-3.533868
1	0.620718	1.507913	-4.887200
1	0.536530	0.103155	-3.782157
6	3.815219	-1.203151	3.046645
1	3.260040	-2.109906	2.770059
1	4.882300	-1.453599	3.028722

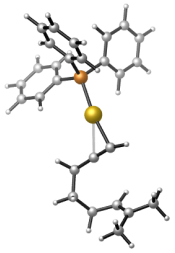
IIa



E = -947.672130 h.
G = -947.399262 h.

6	1.047174	0.951406	1.627963
1	0.243170	1.484049	2.145964
6	1.731320	0.046900	2.399130
6	2.928288	-0.751604	1.928098
1	2.630279	-1.757302	1.601483
1	3.335359	-0.247075	1.042305
6	3.358109	-0.061308	4.292395
1	3.384491	-0.683490	5.198088
1	3.926098	0.848551	4.515470
6	1.930793	0.330061	3.991848
1	1.600158	1.324686	4.291737
6	0.901664	-0.623367	3.703498
6	1.103891	-2.110670	3.804862
1	0.697437	-2.433395	4.773858
1	0.539060	-2.635440	3.023892
1	2.145726	-2.437199	3.765514
6	-0.538390	-0.216857	3.873829
1	-1.179092	-0.667942	3.105880
1	-0.879431	-0.588592	4.850018
1	-0.684791	0.868273	3.873421
79	1.361581	1.394563	-0.356383
15	1.712673	1.980180	-2.629766
6	3.138744	1.158505	-3.413113
1	2.996747	0.071390	-3.396478
1	3.243554	1.492951	-4.453952
1	4.056452	1.398955	-2.862975
6	2.020941	3.758495	-2.886311
1	2.198818	3.963880	-3.950709
1	1.153442	4.337384	-2.547165
1	2.898026	4.072903	-2.308143
6	0.317219	1.605453	-3.739944
1	-0.576640	2.149193	-3.411424
1	0.562606	1.900736	-4.768933
1	0.099219	0.530983	-3.717422
6	3.953115	-0.804036	3.075154
1	4.203227	-1.839803	3.334077
1	4.893538	-0.328510	2.773165

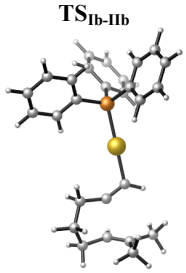
Ib



E = -1522.416687 h.
G = -1522.004912 h.

6	0.715254	0.483206	1.059169
1	-0.300325	0.756489	1.294772
6	1.856401	0.023140	1.123719
6	3.188337	-0.565436	1.223509
1	3.397677	-1.094876	0.282592
1	3.934429	0.240327	1.306551
6	3.418580	-0.862941	3.770601
1	3.606449	-1.642711	4.522871
1	4.301992	-0.206490	3.783070
6	2.194956	-0.066700	4.118323
1	2.224693	0.998846	3.869807
6	1.059191	-0.544307	4.647776
6	0.849047	-1.976224	5.033756
1	0.468741	-2.049656	6.063854
1	0.085127	-2.443596	4.392866
1	1.758567	-2.584157	4.964885
6	-0.125854	0.344057	4.869431
1	-1.006045	-0.032328	4.324152
1	-0.415586	0.367906	5.931406
1	0.063325	1.375493	4.543978
79	1.458081	1.271456	-0.897027
15	1.860384	2.245380	-2.981174
6	3.333314	-1.541516	2.402613
1	2.493842	-2.252454	2.389576
1	4.248678	-2.121389	2.222934
6	3.611045	2.096821	-3.448248
6	4.275130	0.896846	-3.168128
6	4.283354	3.129815	-4.106064
6	5.601404	0.732023	-3.549064
1	3.748534	0.090034	-2.653437
6	5.613877	2.960750	-4.479055
1	3.771151	4.066084	-4.328408
6	6.271046	1.765524	-4.201543
1	6.116399	-0.201885	-3.331207
1	6.137132	3.767746	-4.988585
1	7.312338	1.638700	-4.492369
6	0.890914	1.468886	-4.306315
6	1.420613	1.258612	-5.582005
6	-0.436397	1.120938	-4.032545
6	0.623364	0.697095	-6.575570
1	2.452415	1.532756	-5.802275
6	-1.228944	0.566918	-5.030690
1	-0.847638	1.286416	-3.034941
6	-0.697097	0.352201	-6.300550
1	1.037602	0.530716	-7.568258
1	-2.261116	0.296623	-4.815682
1	-1.316003	-0.088975	-7.079860
6	1.458212	4.016400	-3.002201
6	1.766429	4.779135	-1.870191
6	0.896428	4.629229	-4.125314
6	1.518713	6.146636	-1.864802
1	2.203126	4.297423	-0.993085
6	0.645030	5.998053	-4.111144
1	0.654280	4.042657	-5.011632
6	0.955328	6.754940	-2.984588
1	1.759909	6.737230	-0.982871
1	0.203311	6.473780	-4.984846
1	0.753428	7.824598	-2.977367

$TS_{Ib\text{-}IIb}$

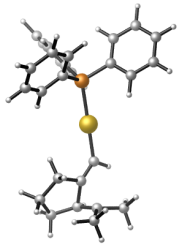


E = -1522.407096 h.
G = -1521.993064 h.

6	1.360303	-0.376681	1.050107
1	1.141704	-1.441348	1.096497
6	1.463101	0.473608	2.004164
6	1.687579	1.880804	2.399013
1	2.377018	2.320195	1.663787
1	0.729761	2.420882	2.323359
6	1.288842	1.216568	4.724538
1	1.745892	1.050736	5.710020

1	0.373317	1.799340	4.890652
6	0.922070	-0.084631	4.067022
1	-0.126753	-0.240233	3.802930
6	1.740839	-1.178916	4.003066
6	3.157146	-1.190066	4.463545
1	3.367596	-2.124380	5.001760
1	3.832427	-1.178591	3.593759
1	3.418772	-0.346444	5.110306
6	1.242706	-2.458794	3.439456
1	1.930313	-2.846596	2.671798
1	1.220987	-3.218681	4.235340
1	0.232872	-2.374951	3.021838
79	1.576344	0.502816	-0.856644
15	1.755351	1.486521	-2.985567
6	2.232060	1.998878	3.812794
1	3.246079	1.576979	3.849994
1	2.303043	3.052050	4.108674
6	2.967451	0.664754	-4.065709
6	4.164284	0.220579	-3.492246
6	2.748596	0.498013	-5.435503
6	5.134631	-0.381741	-4.284827
1	4.332837	0.347346	-2.421022
6	3.720735	-0.112466	-6.223172
1	1.820714	0.844871	-5.890405
6	4.910795	-0.551461	-5.649634
1	6.063852	-0.727848	-3.835722
1	3.545715	-0.244856	-7.289399
1	5.667297	-1.031029	-6.268375
6	2.264268	3.231764	-2.889251
6	3.107303	3.812663	-3.840450
6	1.758040	4.009798	-1.841459
6	3.440142	5.160785	-3.740814
1	3.505341	3.215494	-4.661042
6	2.086234	5.357630	-1.751943
1	1.102418	3.555598	-1.095016
6	2.930566	5.932081	-2.699898
1	4.101328	5.608406	-4.480659
1	1.689141	5.959385	-0.936407
1	3.194433	6.985613	-2.625397
6	0.173640	1.463663	-3.885293
6	-0.240536	2.525301	-4.694006
6	-0.623516	0.318592	-3.776535
6	-1.444942	2.438010	-5.386683
1	0.375184	3.420191	-4.785694
6	-1.821217	0.233552	-4.476871
1	-0.300959	-0.508035	-3.140482
6	-2.232999	1.295304	-5.279754
1	-1.767025	3.267962	-6.013126
1	-2.437495	-0.659555	-4.391327
1	-3.174794	1.232880	-5.822193

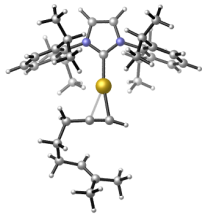
IIb



E = -1522.431515 h.
G = -1522.012590 h.

6	0.966320	0.915805	1.590677
1	0.046414	1.227587	2.095294
6	1.842990	0.193950	2.358271
6	3.211288	-0.263918	1.895684
1	3.167185	-1.270149	1.456458
1	3.529152	0.411713	1.090651
6	3.391566	0.360157	4.303643
1	3.545096	-0.247141	5.206509
1	3.720975	1.377487	4.543509
6	1.920251	0.411769	3.964832
1	1.351897	1.278346	4.303255
6	1.155795	-0.741375	3.594986
6	1.696892	-2.143717	3.623757
1	1.364362	-2.598273	4.568050
1	1.271753	-2.742400	2.808298
1	2.785805	-2.221495	3.591258
6	-0.343692	-0.697645	3.724865
1	-0.838972	-1.218939	2.896296
1	-0.613114	-1.222070	4.652044
1	-0.741755	0.318978	3.801752
79	1.212711	1.394025	-0.390130
15	1.521375	1.928015	-2.690499
6	4.170971	-0.203799	3.096547
1	4.578325	-1.195932	3.324253
1	5.033480	0.434701	2.873370
6	1.989624	3.668303	-2.949045
6	1.381333	4.635920	-2.141459
6	2.900212	4.058516	-3.935086
6	1.676239	5.982307	-2.324131
1	0.674953	4.329111	-1.367733
6	3.197375	5.407365	-4.108673
1	3.377067	3.312069	-4.570793
6	2.586822	6.367220	-3.305738
1	1.200861	6.731629	-1.693705
1	3.908043	5.709253	-4.875927
1	2.823479	7.420877	-3.443880
6	0.036574	1.642991	-3.703650
6	-0.280410	2.450687	-4.799168
6	-0.775137	0.547523	-3.388478
6	-1.400483	2.160545	-5.572737
1	0.346989	3.305477	-5.052552
6	-1.889331	0.258243	-4.168392
1	-0.530220	-0.077941	-2.527537
6	-2.202211	1.065932	-5.259498
1	-1.647180	2.791146	-6.425084
1	-2.516891	-0.595752	-3.919735
1	-3.077996	0.841580	-5.866057
6	2.845699	0.931813	-3.447528
6	4.019813	0.738104	-2.709584
6	2.732349	0.381488	-4.726245
6	5.070924	0.006912	-3.250020
1	4.109557	1.166840	-1.709133
6	3.784725	-0.358622	-5.259350
1	1.823411	0.527575	-5.309414
6	4.951387	-0.545403	-4.524028
1	5.983156	-0.139444	-2.674340
1	3.690093	-0.789586	-6.254552
1	5.771368	-1.125224	-4.944183

Ic

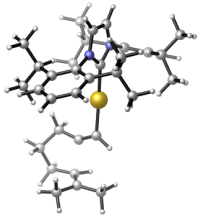


E = -1645.880563 h.

G = -1645.180787 h.

6	2.596790	-0.000699	0.916876
1	3.226126	-0.834026	0.650876
6	1.785765	0.739448	1.478460
6	0.841185	1.572418	2.220368
1	1.297803	2.564800	2.354896
1	-0.062113	1.724054	1.607317
6	-0.570426	-0.150895	3.506520
1	-0.826013	-0.448846	4.533657
1	-1.496911	0.246405	3.063565
6	-0.099664	-1.330084	2.706644
1	-0.356950	-1.323008	1.642406
6	0.645472	-2.351517	3.152723
6	1.095532	-2.509203	4.572141
1	0.792310	-3.490173	4.968905
1	2.194421	-2.481691	4.635259
1	0.703698	-1.737143	5.244317
6	1.116710	-3.430062	2.226419
1	2.217186	-3.482202	2.213665
1	0.769193	-4.421236	2.556920
1	0.770753	-3.273042	1.196425
79	2.588382	1.716198	-0.490166
6	2.804207	3.110983	-1.971766
7	2.217961	4.326384	-2.004191
7	3.538329	3.034984	-3.099706
6	3.415459	4.198414	-3.842437
1	3.930209	4.325315	-4.786427
6	2.585585	5.015871	-3.148296
1	2.218634	6.014024	-3.351177
6	1.370538	4.823933	-0.955427
6	-0.012775	4.612620	-1.056474
6	-0.804809	5.069994	-0.001675
6	1.139367	5.895732	1.165638
6	-0.235397	5.705904	1.095927
1	-1.883599	4.921366	-0.038817
1	1.572868	6.394641	2.032426
1	-0.871796	6.057226	1.906781
6	4.326417	1.887161	-3.455574
6	3.718555	0.875364	-4.210816
6	5.648966	1.820639	-2.993469
6	4.493485	-0.247255	-4.510686
6	6.375989	0.672433	-3.313032
6	5.805474	-0.348271	-4.064935
1	4.058812	-1.055052	-5.099271
1	7.404295	0.574948	-2.966054
1	6.391799	-1.233411	-4.307321
6	-0.630935	3.865570	-2.219684
1	0.106047	3.825061	-3.036439
1	5.598251	3.787727	-2.164914
6	6.267505	2.913376	-2.147027
6	2.285580	0.965799	-4.692139
1	1.851661	1.908828	-4.324877
6	0.453248	0.983283	3.586087
1	1.359294	0.635459	4.105074
1	0.037848	1.805535	4.184178
6	1.977765	5.454225	0.139169
6	3.474845	5.661371	0.237952
1	3.950397	5.222062	-0.652820
6	3.818362	7.148843	0.251898
1	3.429236	7.657750	-0.640819
1	3.396024	7.648263	1.135366
1	4.907002	7.291654	0.277024
6	4.052403	4.950245	1.459797
1	5.142614	5.080186	1.499557
1	3.637124	5.353274	2.394483
1	3.840333	3.869311	1.435529
6	-1.877150	4.556148	-2.765137
1	-2.705056	4.530278	-2.043461
1	-1.682828	5.606263	-3.020203
1	-2.221849	4.044125	-3.673220
6	-0.955960	2.426985	-1.812461
1	-1.699837	2.413391	-1.001834
1	-1.374840	1.869434	-2.662076
1	-0.060247	1.888142	-1.460762
6	6.388748	2.456452	-0.693633
1	7.063015	1.591547	-0.607819
1	6.796119	3.261850	-0.066772
1	5.409975	2.161468	-0.281860
6	7.621303	3.364827	-2.687037
1	8.375238	2.568369	-2.616624
1	7.555687	3.673755	-3.738652
1	7.993354	4.218549	-2.105025
6	2.225554	0.996113	-6.217274
1	2.811700	1.830811	-6.625901
1	2.619293	0.065368	-6.649854
1	1.188285	1.109515	-6.560142
6	1.439882	-0.174173	-4.129695
1	0.397047	-0.077193	-4.461097
1	1.804591	-1.152671	-4.472485
1	1.448229	-0.177860	-3.028930

$TS_{Ic\text{-}IIc}$

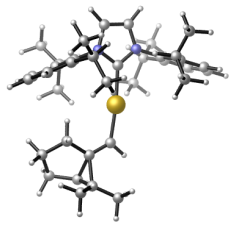


E = -1645.866076 h.
G = -1645.164241 h.

6	0.968811	0.239016	0.770198
1	0.315501	-0.526084	0.354067
6	1.347488	0.360538	1.992875
6	2.102984	1.162557	2.979991
1	2.924674	1.657617	2.441969
1	1.441789	1.952383	3.372808
6	1.409457	-0.436623	4.691100
1	1.725935	-1.263736	5.341746
1	0.816720	0.247917	5.311824
6	0.549564	-0.929927	3.559217
1	-0.461630	-0.523526	3.476957
6	0.828239	-2.038963	2.805342
6	2.099471	-2.808707	2.889991
1	1.890677	-3.886052	2.843824
1	2.725864	-2.578755	2.013915
1	2.683014	-2.601333	3.792401
6	-0.156153	-2.538188	1.813592
1	0.317063	-2.706745	0.834015
1	-0.526301	-3.521226	2.142445
1	-1.019107	-1.872628	1.699809
79	1.740910	1.681871	-0.546490
6	2.561688	3.073537	-1.832351
7	2.121623	4.320053	-2.115054
7	3.730471	2.958059	-2.502869
6	4.019852	4.118455	-3.202290
1	4.912906	4.207929	-3.808104
6	2.999984	4.978258	-2.961104
1	2.810556	5.988309	-3.301914
6	0.885998	4.859900	-1.620418
6	-0.283157	4.612665	-2.351976

6	-1.479362	5.110282	-1.830468
6	-0.318626	6.045275	0.066707
6	-1.497974	5.814300	-0.632827
1	-2.409618	4.940112	-2.372853
1	-0.347869	6.599059	1.004701
1	-2.441475	6.192169	-0.241671
6	4.528786	1.764942	-2.514814
6	4.330496	0.848973	-3.556972
6	5.447886	1.561239	-1.474912
6	5.112470	-0.308188	-3.548387
6	6.212009	0.394376	-1.519427
6	6.046972	-0.530281	-2.545048
1	4.984376	-1.046436	-4.340179
1	6.947978	0.206108	-0.738588
1	6.652535	-1.435245	-2.559179
6	-0.280351	3.857723	-3.665058
1	0.751386	3.544295	-3.887405
1	4.750757	3.221926	-0.332557
6	5.638852	2.571744	-0.363152
6	3.312320	1.071988	-4.655781
1	2.826951	2.046164	-4.492307
6	2.617020	0.308377	4.124663
1	3.368694	-0.397688	3.743526
1	3.104464	0.930300	4.884405
6	0.904074	5.573439	-0.412889
6	2.180124	5.787421	0.375274
1	3.033237	5.560483	-0.282847
6	2.219515	0.006143	-4.615149
1	1.471244	0.191914	-5.398242
1	2.635079	-0.998114	-4.781787
1	1.699870	-0.000876	-3.645276
6	3.983223	1.121258	-6.026236
1	4.756903	1.900588	-6.067013
1	4.459639	0.162456	-6.275226
1	3.243371	1.336236	-6.809065
6	5.763197	1.917532	1.009302
1	6.704526	1.360147	1.116380
1	5.751909	2.686180	1.794255
1	4.935723	1.217963	1.202507
6	6.848889	3.456883	-0.658637
1	7.768505	2.855532	-0.710831
1	6.736559	3.982437	-1.617303
1	6.983020	4.211358	0.128739
6	2.341289	7.226558	0.853544
1	2.269329	7.942970	0.024489
1	1.580942	7.495286	1.600016
1	3.322493	7.356661	1.329669
6	2.238896	4.818515	1.556561
1	3.190462	4.921737	2.097864
1	1.421573	5.016565	2.266217
1	2.142680	3.774933	1.217749
6	-0.739359	4.762251	-4.806783
1	-1.781301	5.083643	-4.667113
1	-0.116438	5.664818	-4.877511
1	-0.679747	4.231389	-5.766541
6	-1.133292	2.594010	-3.589114
1	-2.183829	2.829359	-3.366501
1	-1.109910	2.061551	-4.549902
1	-0.768575	1.906354	-2.811493

IIc

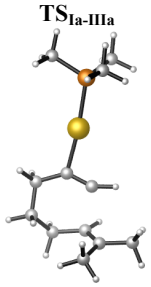


E = -1645.895359 h.
G = -1645.187511 h.

6	1.059021	0.751157	1.367650
1	0.198786	0.984955	2.003148
6	1.699521	-0.433129	1.657114
6	2.949698	-0.911066	0.939391
1	2.697417	-1.563975	0.090907
1	3.446534	-0.029135	0.509199
6	3.204826	-1.472069	3.351128
1	3.203384	-2.422560	3.902929
1	3.749799	-0.746161	3.966087
6	1.789406	-0.972969	3.185288
1	1.416192	-0.258652	3.919730
6	0.796166	-1.633858	2.387639
6	0.988929	-2.982441	1.747423
1	0.538699	-3.732767	2.412743
1	0.454869	-3.033115	0.789864
1	2.029094	-3.273288	1.586087
6	-0.654936	-1.329096	2.657141
1	-1.244044	-1.314836	1.731631
1	-1.054148	-2.131448	3.292964
1	-0.807369	-0.387394	3.194604
79	1.659930	2.028974	-0.104827
6	2.469722	3.278908	-1.554871
7	2.034753	4.447552	-2.075025
7	3.671049	3.065425	-2.142534
6	3.988814	4.090789	-3.016144
1	4.914926	4.094241	-3.576852
6	2.950286	4.961905	-2.978877
1	2.773393	5.896440	-3.496242
6	0.761222	5.041418	-1.779835
6	-0.343767	4.649895	-2.548928
6	-1.567900	5.257888	-2.261652
6	-0.564039	6.552148	-0.490030
6	-1.676838	6.197588	-1.244037
1	-2.448654	4.990232	-2.845061
1	-0.668122	7.286118	0.308295
1	-2.640579	6.660274	-1.036371
6	4.483113	1.908118	-1.886615
6	4.329825	0.792936	-2.725266
6	5.357168	1.930599	-0.791984
6	5.106076	-0.331877	-2.441634
6	6.111993	0.779349	-0.552059
6	5.990768	-0.337944	-1.368857
1	5.012992	-1.219427	-3.066546
1	6.805658	0.762141	0.289016
1	6.587268	-1.225703	-1.163008
6	-0.237594	3.629598	-3.664531
1	0.759823	3.164065	-3.619086
1	4.798098	3.911795	-0.219914
6	5.491362	3.128418	0.124490
6	3.302828	0.759834	-3.837798
1	2.994988	1.793681	-4.058217
6	3.857434	-1.615936	1.961470
1	4.002932	-2.671821	1.704354

1	4.857755	-1.165075	1.966919
6	0.685597	5.984907	-0.745024
6	1.888493	6.343285	0.102220
1	2.794994	6.013239	-0.429027
6	2.017734	7.845003	0.335503
1	2.020143	8.405398	-0.608831
1	1.199271	8.233421	0.957422
1	2.955967	8.064895	0.862069
6	1.832998	5.596858	1.435724
1	2.722312	5.821426	2.041584
1	0.945996	5.896256	2.013681
1	1.782666	4.505830	1.287498
6	-0.367417	4.305953	-5.027924
1	-1.357290	4.769838	-5.147211
1	0.389280	5.091272	-5.162783
1	-0.242535	3.571772	-5.835578
6	-1.263826	2.510911	-3.509272
1	-2.292315	2.887086	-3.600594
1	-1.121962	1.752946	-4.292051
1	-1.171380	2.012245	-2.533694
6	3.844893	0.160247	-5.130612
1	4.760005	0.668245	-5.462414
1	4.070625	-0.909759	-5.022540
1	3.096545	0.252850	-5.928973
6	2.060698	-0.002587	-3.371239
1	1.277137	0.021822	-4.141799
1	2.305165	-1.057296	-3.172920
1	1.647015	0.423909	-2.442524
6	6.903991	3.704266	0.064767
1	7.645876	2.979186	0.428849
1	7.179232	3.980130	-0.962659
1	6.980216	4.603606	0.690848
6	5.101742	2.767670	1.557243
1	5.772608	2.003385	1.976390
1	5.159136	3.652387	2.206287
1	4.071515	2.378090	1.606276

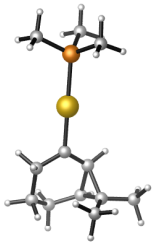
$TS_{Ia\text{-}IIIa}$



E = -947.642063 h.
G = -947.373726 h.

6	1.356208	0.491400	1.981972
1	0.335343	0.839073	2.020671
6	2.472133	0.323871	1.401771
6	3.802658	-0.229371	1.776550
1	4.221303	-0.793817	0.933178
1	4.485619	0.620535	1.936844
6	3.162667	-0.385233	4.254079
1	3.258025	-1.064033	5.115612
1	3.806401	0.477945	4.477298
6	1.735097	0.099417	4.174080
1	1.576669	1.169101	4.333857
6	0.623410	-0.685434	4.161822
6	0.659101	-2.175053	4.076403
1	-0.118706	-2.608604	4.720018
1	0.433081	-2.507089	3.050960
1	1.624777	-2.602819	4.367471
6	-0.739676	-0.081358	4.208742
1	-1.346600	-0.412416	3.350850
1	-1.273566	-0.421531	5.108120
1	-0.713640	1.015343	4.220773
79	2.081662	1.145609	-0.545426
15	1.871478	1.986137	-2.722549
6	3.388650	1.788254	-3.707588
1	3.640758	0.724731	-3.794699
1	3.246621	2.210021	-4.711708
1	4.220155	2.305067	-3.213645
6	1.503094	3.766943	-2.803108
1	1.440520	4.091050	-3.850598
1	0.549489	3.974319	-2.303327
1	2.294727	4.331801	-2.296611
6	0.566342	1.197225	-3.715393
1	-0.408554	1.348243	-3.236564
1	0.545338	1.631569	-4.723943
1	0.756430	0.120013	-3.789880
6	3.724268	-1.100523	3.021138
1	3.126801	-1.994483	2.791644
1	4.736484	-1.452998	3.260121

IIIa

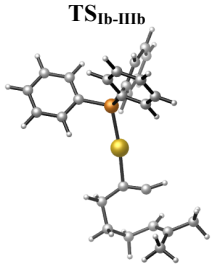


E = -947.680722 h.
G = -947.407488 h.

6	1.333727	0.547909	2.521638
1	0.589862	1.309065	2.289960
6	2.282274	0.227228	1.545884
6	3.493794	-0.569030	1.863281
1	3.490926	-1.447579	1.192504
1	4.327649	0.030481	1.456073
6	3.176805	0.005968	4.308359
1	3.251550	-0.400572	5.326930
1	3.753329	0.943168	4.303469
6	1.738585	0.363352	4.035357
1	1.370458	1.211567	4.617018
6	0.704020	-0.535915	3.563011
6	0.854319	-2.014804	3.292256
1	1.060285	-2.542729	4.234114
1	-0.089325	-2.408349	2.893967
1	1.638389	-2.275474	2.578300
6	-0.717758	-0.159545	3.897582
1	-1.397637	-0.410890	3.073627
1	-1.033828	-0.737418	4.778136
1	-0.825381	0.905947	4.133357
79	2.085490	0.992320	-0.371197
15	1.856054	1.885279	-2.558874
6	3.286673	1.611460	-3.653198
1	3.455987	0.536239	-3.786702
1	3.108089	2.072622	-4.634059
1	4.186690	2.052460	-3.207996
6	1.612870	3.691733	-2.586070
1	1.522651	4.047485	-3.621215
1	0.702067	3.953901	-2.034402
1	2.464284	4.189575	-2.106629
6	0.440277	1.230265	-3.500885
1	-0.491543	1.424305	-2.956307

1	0.387656	1.709281	-4.487850
1	0.547405	0.146846	-3.631971
6	3.781134	-0.973174	3.311080
1	3.418865	-1.987033	3.513772
1	4.867873	-1.013037	3.456611

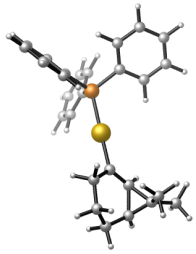
$TS_{Ib\text{-}IIIb}$



E = -1522.400424 h.
G = -1521.987861 h.

6	1.360648	0.487342	1.914828
1	0.340974	0.836035	1.969688
6	2.474093	0.319598	1.331397
6	3.806172	-0.239974	1.690245
1	4.216418	-0.796836	0.837718
1	4.492039	0.607049	1.853117
6	3.189213	-0.419568	4.173103
1	3.290463	-1.108871	5.025556
1	3.839315	0.437995	4.399456
6	1.763294	0.072408	4.112841
1	1.612008	1.142292	4.278269
6	0.647782	-0.706117	4.102060
6	0.674963	-2.195341	4.004796
1	-0.097816	-2.630159	4.653639
1	0.436103	-2.518283	2.979338
1	1.641580	-2.630357	4.281728
6	-0.712212	-0.096076	4.165025
1	-1.328262	-0.418830	3.310481
1	-1.239792	-0.439637	5.066842
1	-0.681261	1.000413	4.183794
79	2.080285	1.166501	-0.598364
15	1.868593	2.039655	-2.771811
6	3.735108	-1.123540	2.926513
1	3.131718	-2.012458	2.693054
1	4.748145	-1.482952	3.151308
6	3.404181	1.830660	-3.723345
6	4.113114	0.632987	-3.575575
6	3.861168	2.803587	-4.615727
6	5.266531	0.409839	-4.318308
1	3.755097	-0.126396	-2.877420
6	5.021345	2.577999	-5.351366
1	3.313724	3.737891	-4.740209
6	5.722250	1.384349	-5.203976
1	5.813499	-0.523874	-4.200717
1	5.378326	3.338722	-6.043307
1	6.629936	1.211602	-5.779648
6	0.555816	1.228240	-3.735896
6	0.718943	0.899733	-5.083992
6	-0.657689	0.956335	-3.093937
6	-0.325264	0.296807	-5.780403
1	1.659594	1.112542	-5.592188
6	-1.698766	0.360779	-3.795906
1	-0.784704	1.214491	-2.040862
6	-1.530526	0.027090	-5.138575
1	-0.194467	0.037662	-6.829497
1	-2.640890	0.150366	-3.292801
1	-2.342831	-0.448870	-5.685073
6	1.487986	3.818359	-2.779762
6	0.672855	4.393847	-3.758649
6	2.063765	4.623787	-1.790725
6	0.437335	5.765484	-3.744378
1	0.221444	3.773869	-4.533380
6	1.830736	5.994314	-1.785834
1	2.697213	4.173374	-1.024112
6	1.014713	6.564116	-2.760693
1	-0.201339	6.210583	-4.505186
1	2.280474	6.617626	-1.015160
1	0.824760	7.635981	-2.751538

IIIb

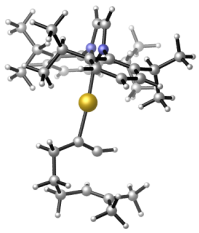


E = -1522.439721 h.
G = -1522.020943 h.

6	1.287445	0.562455	2.465802
1	0.525041	1.300999	2.221592
6	2.276447	0.290146	1.516638
6	3.505478	-0.468816	1.856667
1	3.549164	-1.338176	1.175488
1	4.330165	0.162608	1.480752
6	3.094105	0.058321	4.299315
1	3.154121	-0.360305	5.313882
1	3.635061	1.016240	4.324344
6	1.652755	0.367821	3.988657
1	1.239233	1.195407	4.569497
6	0.662434	-0.557048	3.473818
6	0.863143	-2.025752	3.185788
1	1.011631	-2.565339	4.132028
1	-0.041878	-2.430182	2.715326
1	1.701083	-2.261678	2.526888
6	-0.780633	-0.230293	3.767860
1	-1.424990	-0.487044	2.917381
1	-1.107361	-0.833889	4.626890
1	-0.930074	0.826683	4.018492
79	2.104937	1.068762	-0.392906
15	1.886006	1.945462	-2.598462
6	3.764458	-0.882540	3.307406
1	3.436202	-1.912422	3.486056
1	4.847089	-0.883040	3.485320
6	0.429486	1.274985	-3.464862
6	0.462752	0.896954	-4.809443
6	-0.764438	1.168618	-2.741575
6	-0.691200	0.415450	-5.422187
1	1.387409	0.976903	-5.381190
6	-1.915028	0.694457	-3.360009
1	-0.789225	1.461325	-1.690120
6	-1.877225	0.315565	-4.700639
1	-0.662167	0.119608	-6.469372
1	-2.841881	0.615151	-2.794689
1	-2.776638	-0.063109	-5.183263
6	1.683989	3.754307	-2.614790
6	0.969993	4.406802	-3.624815
6	2.291588	4.500667	-1.599666
6	0.869516	5.794270	-3.617622
1	0.493833	3.832232	-4.419927
6	2.190855	5.887975	-1.598557

1	2.840637	3.989011	-0.806773
6	1.479084	6.533542	-2.606690
1	0.313760	6.299748	-4.405339
1	2.664516	6.464697	-0.806138
1	1.395613	7.618910	-2.602712
6	3.315080	1.570485	-3.662131
6	3.823381	2.488577	-4.584017
6	3.886540	0.296530	-3.561781
6	4.897291	2.133450	-5.395833
1	3.381862	3.481150	-4.673161
6	4.954020	-0.055657	-4.379827
1	3.488186	-0.421181	-2.841650
6	5.461177	0.864882	-5.294730
1	5.293857	2.852366	-6.110677
1	5.395605	-1.047269	-4.297599
1	6.303083	0.592206	-5.928787

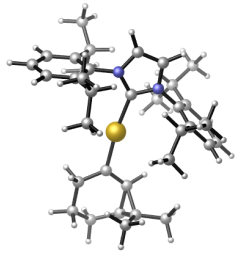
$TS_{Ic\text{-}IIIc}$



E = -1645.862104 h.
G = -1645.162271 h.

6	2.150688	-0.075574	1.521037
1	3.168985	0.044319	1.859551
6	1.178835	0.194790	0.748444
6	-0.211252	-0.302663	0.560175
1	-0.882844	0.542721	0.356509
1	-0.221370	-0.919071	-0.353931
6	0.202459	-2.291754	2.117326
1	-0.306821	-2.887194	2.890991
1	0.280863	-2.946845	1.237526
6	1.598328	-1.968934	2.595139
1	2.418041	-2.451396	2.056498
6	1.920341	-1.345122	3.761319
6	0.915077	-0.754044	4.693944
1	1.226885	-0.914250	5.735145
1	0.850801	0.336416	4.553792
1	-0.089671	-1.172429	4.567338
6	3.343438	-1.191374	4.181509
1	3.582997	-0.132745	4.370166
1	3.514863	-1.715103	5.133457
1	4.048606	-1.589348	3.441389
79	2.045874	1.695556	-0.489822
6	2.740046	3.144456	-1.774614
7	2.512339	4.474868	-1.721105
7	3.525857	2.966556	-2.858664
6	3.791926	4.174421	-3.481722
1	4.406464	4.228694	-4.371553
6	3.153813	5.128975	-2.760217
1	3.085292	6.202393	-2.881728
6	1.695105	5.108931	-0.724273
6	0.331880	5.287555	-1.001567
6	-0.445437	5.894723	-0.013682
6	1.471953	6.102232	1.435992
6	0.118852	6.300666	1.190083
1	-1.510243	6.046747	-0.187750
1	1.897168	6.417873	2.388538
1	-0.504767	6.774389	1.946744
6	3.981088	1.680886	-3.305643
6	3.141512	0.937469	-4.146738
6	5.223250	1.217973	-2.850045
6	3.591065	-0.323713	-4.543263
6	5.625745	-0.049143	-3.275912
6	4.819484	-0.811018	-4.113411
1	2.967382	-0.933503	-5.197029
1	6.583442	-0.448369	-2.942331
1	5.152998	-1.796646	-4.434834
6	-0.301597	4.796749	-2.287078
1	0.501615	4.545301	-2.996635
1	5.648506	3.022401	-1.791063
6	6.092120	2.022197	-1.905405
6	1.793408	1.447120	-4.613063
1	1.636053	2.455131	-4.198310
6	-0.697497	-1.104613	1.757432
1	-0.802553	-0.430051	2.619066
1	-1.702352	-1.487205	1.534046
6	2.294114	5.498980	0.481611
6	3.756609	5.245781	0.781699
1	4.241290	4.877751	-0.135428
6	4.485216	6.519473	1.199941
1	4.389196	7.306814	0.440178
1	4.098361	6.917265	2.148529
1	5.554742	6.314689	1.343207
6	3.901849	4.159413	1.847547
1	4.962396	3.930218	2.023644
1	3.466036	4.483993	2.803840
1	3.392004	3.229601	1.544572
6	-1.174822	5.858186	-2.948080
1	-2.055149	6.102599	-2.337468
1	-0.618061	6.788290	-3.123662
1	-1.542430	5.494753	-3.917145
6	-1.102556	3.519683	-2.029411
1	-1.936657	3.711030	-1.338074
1	-1.525883	3.133759	-2.967416
1	-0.471896	2.731109	-1.586951
6	7.502184	2.211672	-2.456849
1	8.034771	1.254707	-2.547807
1	7.484409	2.682467	-3.449091
1	8.091472	2.853072	-1.787751
6	6.127472	1.376506	-0.520502
1	6.571968	0.371624	-0.563271
1	6.731487	1.981940	0.169748
1	5.116222	1.281009	-0.092607
6	1.750464	1.566990	-6.134088
1	2.546394	2.227181	-6.505870
1	1.872525	0.587098	-6.617449
1	0.786525	1.979819	-6.461010
6	0.662819	0.559139	-4.097669
1	-0.311786	0.952044	-4.418956
1	0.751939	-0.466059	-4.484701
1	0.663987	0.506272	-2.996861

IIIc

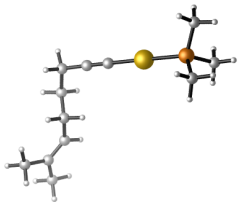


E = -1645.902799 h.
G = -1645.194010 h.

6	1.501785	-1.076574	0.711972

1	1.827853	-1.233678	-0.317504
6	1.128748	0.225715	1.091213
6	0.345780	0.468607	2.325035
1	0.810204	1.301528	2.880553
1	-0.573157	0.942067	1.925604
6	-0.146713	-2.018010	2.496876
1	-0.211399	-2.849674	3.212587
1	-1.088698	-2.023827	1.927829
6	0.964329	-2.295563	1.514871
1	0.771279	-3.141197	0.850814
6	2.380281	-2.003918	1.710906
6	3.016522	-1.414538	2.948704
1	2.944260	-2.135409	3.775783
1	4.084075	-1.238554	2.761682
1	2.588411	-0.467448	3.284959
6	3.355300	-2.834170	0.914576
1	4.197906	-2.222137	0.564530
1	3.765796	-3.620928	1.564223
1	2.886287	-3.316246	0.048232
79	1.713345	1.754891	-0.140123
6	2.545095	3.161493	-1.423452
7	2.390807	4.499736	-1.518899
7	3.491684	2.855218	-2.339455
6	3.928177	3.987513	-3.004361
1	4.686094	3.938497	-3.776514
6	3.230325	5.029107	-2.485670
1	3.242376	6.088494	-2.707971
6	1.440331	5.248117	-0.744135
6	0.144255	5.397700	-1.258543
6	-0.774422	6.100420	-0.476273
6	0.887138	6.461732	1.236556
6	-0.407144	6.625795	0.756783
1	-1.794445	6.232955	-0.835740
1	1.157623	6.874894	2.207766
1	-1.139138	7.169900	1.351822
6	3.938415	1.512088	-2.581906
6	3.252218	0.749913	-3.537780
6	4.998111	1.008552	-1.814842
6	3.687617	-0.560724	-3.743931
6	5.393537	-0.308533	-2.058115
6	4.749863	-1.083316	-3.016129
1	3.182315	-1.180264	-4.484770
1	6.218021	-0.731847	-1.483649
1	5.075748	-2.107279	-3.193329
6	-0.276244	4.788763	-2.580423
1	0.627371	4.445209	-3.107149
1	5.202006	2.804414	-0.673756
6	5.687079	1.818431	-0.737360
6	2.059375	1.282061	-4.303912
1	1.871697	2.319696	-3.987126
6	-0.013053	-0.697096	3.246431
1	0.728871	-0.795246	4.047318
1	-0.961170	-0.470779	3.751026
6	1.844638	5.768248	0.493481
6	3.241072	5.553939	1.038798
1	3.875896	5.184904	0.219019
6	-0.974624	5.797383	-3.487629
1	-1.938878	6.121860	-3.072297
1	-0.358876	6.692167	-3.648879
1	-1.177865	5.345173	-4.467624
6	-1.163635	3.566486	-2.346076
1	-2.098425	3.850244	-1.840405
1	-1.430518	3.093227	-3.301634
1	-0.659232	2.813640	-1.720032
6	3.871288	6.843887	1.555064
1	4.914667	6.661816	1.845497
1	3.864076	7.632756	0.791413
1	3.348899	7.227198	2.442559
6	3.229283	4.485475	2.132713
1	2.629885	4.813234	2.995106
1	2.801683	3.536799	1.767608
1	4.250078	4.285717	2.488615
6	7.156278	2.049305	-1.079869
1	7.702961	1.098001	-1.148215
1	7.265583	2.569301	-2.041761
1	7.642615	2.659050	-0.306475
6	5.536487	1.148040	0.627508
1	6.062136	0.182532	0.659135
1	5.962396	1.782816	1.416827
1	4.475681	0.968596	0.869155
6	2.330954	1.301840	-5.805374
1	3.223347	1.897312	-6.043441
1	2.489080	0.287018	-6.197393
1	1.479037	1.737526	-6.344797
6	0.804551	0.472971	-3.980959
1	-0.067156	0.889697	-4.504182
1	0.910516	-0.574302	-4.298198
1	0.588058	0.477911	-2.900641

VIIa

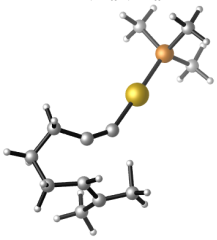


E = -947.213993 h.
G = -946.958202 h.

6	0.014954	1.307518	1.180542
6	1.239292	1.363241	1.250989
6	2.698924	1.421576	1.306403
1	3.063625	0.780951	2.123960
1	3.019398	2.445486	1.561796
79	-2.005407	1.216249	1.059911
15	-4.349120	1.109363	0.898843
6	-5.231810	1.094107	2.495099
1	-6.317150	1.068155	2.327736
1	-4.935118	0.212721	3.076394
1	-4.976668	1.991179	3.071994
6	-5.105662	2.504785	0.000094
1	-4.708482	2.549180	-1.021086
1	-6.197126	2.387603	-0.041423
1	-4.862785	3.446537	0.506692
6	-4.991897	-0.363220	0.036681
1	-6.089932	-0.343174	0.011369
1	-4.607886	-0.389530	-0.990191
1	-4.659768	-1.271306	0.554008
6	3.371775	1.000925	-0.004171
1	4.461698	0.988467	0.147137
1	3.075998	-0.031367	-0.250095
6	3.033021	1.921620	-1.174099
1	1.935265	1.948754	-1.284389
1	3.339992	2.949142	-0.926527
6	5.104340	3.441299	-2.980686
1	4.746858	3.901118	-2.053239
1	6.203750	3.402072	-2.934763
1	4.858899	4.123177	-3.809726
6	5.052969	1.430162	-4.487525
1	6.148982	1.325375	-4.460162
1	4.619850	0.434465	-4.647557
1	4.827316	2.045340	-5.372919
6	3.649181	1.451228	-2.452642

1	3.328607	0.450634	-2.765789
6	4.539391	2.077069	-3.235547

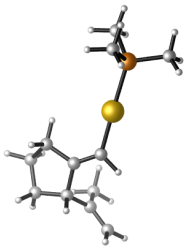
$TS_{VIIa\text{-}VIIIa}$



E = -947.152379 h.
G = -946.896805 h.

6	0.764713	1.993175	-0.724066
6	1.858901	2.289083	-0.136983
6	2.555750	2.381801	1.180619
1	2.026347	1.790334	1.940028
1	2.550325	3.430279	1.526103
79	-1.203075	1.500020	-0.540112
15	-3.472516	0.925535	-0.285340
6	-3.814501	-0.132292	1.161538
1	-4.888431	-0.354024	1.229877
1	-3.257424	-1.072961	1.075358
1	-3.492332	0.377480	2.077656
6	-4.605300	2.336966	-0.050102
1	-4.562987	3.001692	-0.921163
1	-5.635527	1.978478	0.080915
1	-4.307336	2.908592	0.837221
6	-4.221544	0.003302	-1.670900
1	-5.273706	-0.225890	-1.452503
1	-4.165983	0.599289	-2.589860
1	-3.675130	-0.933842	-1.831549
6	3.996714	1.933356	0.988145
1	4.606217	2.088636	1.888509
1	4.011657	0.856576	0.757943
6	4.513920	2.726831	-0.210404
1	4.799095	3.736401	0.119987
1	5.417055	2.268464	-0.637484
6	3.878616	0.618935	-2.356700
1	4.820688	0.564249	-1.795959
1	3.189057	-0.117611	-1.906305
1	4.074421	0.278288	-3.382467
6	2.098638	2.206300	-3.122166
1	1.235163	1.997967	-2.226673
1	1.866794	3.246838	-3.378698
1	1.912787	1.522760	-3.958109
6	3.398134	2.831255	-1.232417
1	3.028074	3.849141	-1.397561
6	3.267998	1.985501	-2.339263

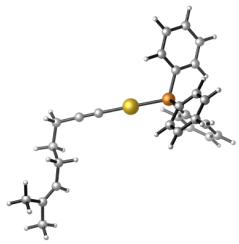
VIIIa



E = -947.230608 h.
G = -946.970704 h.

6	0.648822	2.106319	-1.509281
6	1.733897	2.387897	-0.770291
6	1.857315	2.319866	0.733950
1	1.162802	1.593547	1.178269
1	1.622095	3.305063	1.174989
79	-1.217251	1.550048	-0.829830
15	-3.388640	0.913567	-0.095504
6	-3.444080	-0.372585	1.199680
1	-4.484283	-0.611926	1.460143
1	-2.944117	-1.280913	0.842056
1	-2.920019	-0.020735	2.096669
6	-4.400710	2.261279	0.608375
1	-4.544937	3.047522	-0.142682
1	-5.381548	1.883079	0.927919
1	-3.886657	2.700581	1.471968
6	-4.458648	0.229937	-1.408882
1	-5.442108	-0.044593	-1.003110
1	-4.591803	0.974149	-2.203512
1	-3.988643	-0.659908	-1.845165
6	3.333022	2.007555	0.970710
1	3.673972	2.245510	1.986678
1	3.517639	0.935343	0.803422
6	4.034686	2.840731	-0.103047
1	4.121311	3.880491	0.244882
1	5.052759	2.494435	-0.327939
6	3.871393	0.455249	-2.072416
1	4.667708	0.387289	-1.315746
1	2.985936	-0.037334	-1.644287
1	4.190678	-0.123793	-2.947800
6	3.695538	2.315690	-3.693653
1	0.798794	2.205890	-2.595366
1	3.478119	3.350621	-3.962270
1	4.018172	1.656878	-4.501327
6	3.103366	2.799729	-1.338182
1	3.022508	3.807102	-1.775864
6	3.572785	1.878122	-2.436434

VIIb

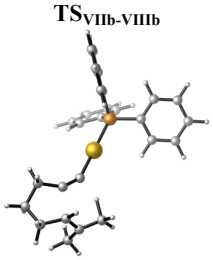


E = -1521.972675 h.
G = -1521.572153 h.

6	-0.087496	1.492789	1.228404
6	1.133598	1.578104	1.317231
6	2.590670	1.667495	1.392753
1	2.951066	1.090023	2.257813
1	2.888973	2.711906	1.583993
79	-2.096010	1.337329	1.071729
15	-4.437247	1.129139	0.873574
6	3.292353	1.171187	0.124302
1	4.379634	1.185584	0.293488
1	3.015550	0.120412	-0.056862
6	2.960984	2.007068	-1.109815
1	1.864793	2.015365	-1.236883
1	3.254884	3.051911	-0.928268
6	5.073789	3.409648	-2.958611
1	4.706145	3.919724	-2.061630
1	6.172334	3.369633	-2.896457
1	4.841054	4.047058	-3.825850
6	5.041886	1.314296	-4.347854

1	6.135527	1.198033	-4.288937
1	4.599770	0.316517	-4.464095
1	4.845369	1.882425	-5.270806
6	3.599220	1.459036	-2.345740
1	3.281274	0.442459	-2.605039
6	4.507408	2.035093	-3.146037
6	-5.221838	2.521015	-0.002664
6	-4.516414	3.119164	-1.052542
6	-6.502537	2.978219	0.320843
6	-5.090228	4.158994	-1.775929
1	-3.512473	2.768749	-1.299048
6	-7.070146	4.023306	-0.401663
1	-7.058347	2.517191	1.137568
6	-6.365998	4.612606	-1.448779
1	-4.536934	4.623067	-2.590490
1	-8.066641	4.378097	-0.143993
1	-6.812749	5.432256	-2.009127
6	-4.925312	-0.374956	-0.034750
6	-5.980224	-0.397885	-0.950253
6	-4.206233	-1.547699	0.224607
6	-6.307432	-1.583723	-1.603042
1	-6.546217	0.509712	-1.160671
6	-4.542347	-2.731024	-0.422631
1	-3.376481	-1.528042	0.933710
6	-5.591664	-2.748198	-1.339036
1	-7.126213	-1.595991	-2.320527
1	-3.978922	-3.639552	-0.217038
1	-5.848031	-3.672173	-1.854845
6	-5.289572	1.029747	2.482029
6	-4.842802	1.870276	3.507893
6	-6.376461	0.180823	2.704913
6	-5.483094	1.866320	4.741860
1	-3.989574	2.528463	3.334640
6	-7.009724	0.174740	3.945001
1	-6.731367	-0.476149	1.910463
6	-6.564697	1.016010	4.961196
1	-5.131601	2.522017	5.536587
1	-7.853851	-0.490903	4.116874
1	-7.060894	1.006751	5.930259

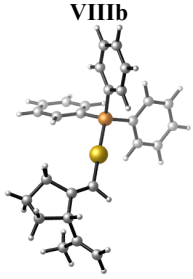
$TS_{VIIb\text{-}VIIIb}$



E = -1521.911479 h.
G = -1521.511711 h.

6	0.760387	1.822647	-0.281503
6	1.944072	1.546970	0.107716
6	2.805204	0.533680	0.787437
1	2.313004	-0.448399	0.796276
1	2.956700	0.828948	1.840317
79	-1.218336	1.358365	-0.281966
15	-3.517624	0.819962	-0.264659
6	4.154258	0.506822	0.084310
1	4.884357	-0.126018	0.606477
1	4.025711	0.096181	-0.929652
6	4.600702	1.965864	0.003227
1	5.034779	2.265276	0.968292
1	5.386243	2.104425	-0.752790
6	3.464437	2.547343	-2.794472
1	4.462350	2.100176	-2.694566
1	2.762704	1.726222	-3.027116
1	3.475082	3.209068	-3.671059
6	1.798900	3.996597	-1.611314
1	1.035848	3.098280	-1.162825
1	1.655827	4.773985	-0.851394
1	1.434712	4.309684	-2.596130
6	3.384263	2.824378	-0.285328
1	3.111643	3.509832	0.524810
6	3.023675	3.271688	-1.560975
6	-4.063836	0.085018	1.312618
6	-3.522182	0.607062	2.492512
6	-5.017854	-0.933795	1.380830
6	-3.940389	0.124034	3.727382
1	-2.769117	1.395597	2.437808
6	-5.427707	-1.420296	2.619472
1	-5.445399	-1.348132	0.467310
6	-4.892112	-0.891489	3.790773
1	-3.516641	0.535386	4.641981
1	-6.169878	-2.215405	2.668807
1	-5.216252	-1.274058	4.757214
6	-4.604892	2.262283	-0.519753
6	-5.842449	2.395132	0.116460
6	-4.175349	3.252384	-1.410439
6	-6.640743	3.506174	-0.140697
1	-6.187460	1.631889	0.814549
6	-4.978082	4.357849	-1.668552
1	-3.204283	3.153483	-1.899234
6	-6.210407	4.485950	-1.031637
1	-7.602941	3.607034	0.358788
1	-4.636182	5.124587	-2.361673
1	-6.835617	5.355183	-1.228991
6	-3.987766	-0.381896	-1.553341
6	-5.209432	-0.322834	-2.229400
6	-3.084292	-1.410365	-1.844020
6	-5.520800	-1.284660	-3.186693
1	-5.920121	0.474614	-2.011461
6	-3.402273	-2.372640	-2.796035
1	-2.126590	-1.451900	-1.321591
6	-4.620319	-2.308196	-3.469268
1	-6.471959	-1.232609	-3.713910
1	-2.694404	-3.169406	-3.017629
1	-4.865909	-3.056572	-4.220948

VIIIb

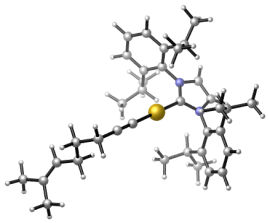


E = -1521.990448 h.
G = -1521.584670 h.

6	0.602797	2.102908	-1.495656
6	1.667769	2.380523	-0.727137
6	1.750235	2.317766	0.780310
1	1.051025	1.585137	1.207458
1	1.490390	3.301628	1.210171
79	-1.275032	1.555150	-0.856179
15	-3.458665	0.910160	-0.133769
6	3.221400	2.021526	1.061608
1	3.530074	2.274300	2.084290

1	3.420843	0.949181	0.912787
6	3.946536	2.849304	-0.000474
1	4.013160	3.893854	0.337386
1	4.973719	2.509938	-0.191996
6	3.842183	0.427185	-1.927889
1	4.617903	0.373929	-1.149049
1	2.945144	-0.057129	-1.514651
1	4.184713	-0.168502	-2.783007
6	3.718679	2.257201	-3.587705
1	0.776475	2.197874	-2.577980
1	3.511221	3.286845	-3.883082
1	4.067778	1.582891	-4.371245
6	3.052598	2.785092	-1.261490
1	2.982979	3.783521	-1.720689
6	3.555118	1.842904	-2.327277
6	-3.441548	-0.375385	1.161096
6	-4.350093	-1.436724	1.183914
6	-2.485787	-0.260887	2.177324
6	-4.299368	-2.373741	2.212698
1	-5.100511	-1.534280	0.399116
6	-2.444953	-1.192966	3.208100
1	-1.772140	0.565528	2.157339
6	-3.349716	-2.252627	3.223324
1	-5.006461	-3.201630	2.224203
1	-1.698788	-1.096876	3.995069
1	-3.311049	-2.988587	4.024874
6	-4.441094	2.279499	0.564844
6	-5.340173	2.100520	1.619833
6	-4.305088	3.542369	-0.022116
6	-6.097875	3.174799	2.077726
1	-5.454667	1.119809	2.082507
6	-5.069094	4.611337	0.433476
1	-3.595896	3.683618	-0.839859
6	-5.964483	4.427644	1.484641
1	-6.797458	3.031254	2.899465
1	-4.958727	5.591296	-0.027901
1	-6.558738	5.265868	1.844842
6	-4.490289	0.221830	-1.473094
6	-5.847880	0.521670	-1.611643
6	-3.881769	-0.660514	-2.373916
6	-6.586592	-0.055895	-2.640969
1	-6.332577	1.207665	-0.916930
6	-4.624927	-1.241537	-3.394960
1	-2.819808	-0.891866	-2.269915
6	-5.977953	-0.936779	-3.530570
1	-7.643432	0.183982	-2.746145
1	-4.145917	-1.927923	-4.091057
1	-6.558262	-1.386315	-4.334638

VIIc



E = -1645.430245 h.
G = -1644.741726 h.

6	-1.199053	1.278009	1.212628
6	0.026307	1.310217	1.287762
6	1.487142	1.336271	1.339178
1	1.838842	0.752092	2.203503
1	1.835959	2.368036	1.513084
79	-3.208166	1.210069	1.039991
6	2.145074	0.797315	0.064357
1	3.235632	0.775106	0.211436
1	1.827097	-0.245210	-0.096001
6	1.818645	1.626780	-1.175447
1	0.721489	1.661373	-1.288421
1	2.141063	2.665887	-1.010656
6	3.929143	2.962801	-3.073324
1	3.588698	3.489281	-2.174795
1	5.027738	2.902176	-3.031938
1	3.691915	3.595750	-3.942677
6	3.834400	0.851877	-4.436027
1	4.926058	0.712290	-4.391224
1	3.369136	-0.137235	-4.534738
1	3.637143	1.413983	-5.362526
6	2.426658	1.049592	-2.413154
1	2.084450	0.036380	-2.654035
6	3.333136	1.597383	-3.235095
6	-5.264643	1.133157	0.832233
6	-7.444123	1.723795	0.698293
1	-8.281886	2.409718	0.703396
6	-7.376572	0.380358	0.533251
1	-8.143654	-0.366795	0.373191
7	-6.141957	2.163699	0.873862
7	-6.036379	0.040401	0.621227
6	-5.515749	-1.293411	0.524077
6	-5.071244	-1.750144	-0.724484
6	-5.450448	-2.064707	1.693173
6	-4.541435	-3.040783	-0.780380
6	-4.911903	-3.347950	1.583387
6	-4.460917	-3.830141	0.360407
1	-4.186165	-3.434451	-1.732525
1	-4.837718	-3.976491	2.470963
1	-4.042102	-4.833325	0.295074
6	-5.758779	3.525953	1.110267
6	-5.479168	4.344260	0.007064
6	-5.659206	3.963147	2.438560
6	-5.083997	5.657183	0.270006
6	-5.272592	5.288616	2.646794
6	-4.985437	6.125198	1.574991
1	-4.845302	6.320772	-0.560528
1	-5.190045	5.670159	3.664322
1	-4.680002	7.154213	1.759186
6	-5.964855	3.056756	3.613310
1	-6.109630	2.032753	3.234116
6	-5.556575	3.832855	-1.416358
1	-6.076282	2.862973	-1.406475
6	-5.168632	-0.911101	-1.981092
1	-5.537248	0.087625	-1.703883
6	-5.900868	-1.533938	3.038113
1	-6.401451	-0.566410	2.880936
6	-6.356338	4.764808	-2.322126
1	-6.472087	4.316715	-3.318271
1	-7.359716	4.958592	-1.919339
1	-5.854475	5.733079	-2.457273
6	-4.156134	3.600404	-1.981571
1	-3.594586	4.544608	-2.039061
1	-3.575301	2.903686	-1.356839
1	-4.215468	3.182242	-2.996398
6	-7.263057	3.478806	4.298104
1	-7.180178	4.491173	4.719643
1	-8.106593	3.475560	3.593364
1	-7.505926	2.793152	5.121580
6	-4.806279	3.007581	4.604999
1	-4.620139	3.989167	5.063294
1	-5.030909	2.304786	5.419063
1	-3.877099	2.678277	4.117521

6	-6.908154	-2.465221	3.706480
1	-7.775577	-2.653560	3.058914
1	-6.457693	-3.436095	3.956468
1	-7.273878	-2.023089	4.643243
6	-4.699053	-1.283753	3.947381
1	-5.027727	-0.877429	4.914349
1	-4.150433	-2.216435	4.144303
1	-3.995146	-0.567365	3.496836
6	-6.175701	-1.517762	-2.955934
1	-5.852899	-2.513318	-3.293442
1	-7.167987	-1.626191	-2.495764
1	-6.281796	-0.882571	-3.846049
6	-3.806409	-0.720375	-2.642558
1	-3.390458	-1.672956	-3.000025
1	-3.894733	-0.052517	-3.510534
1	-3.081724	-0.275339	-1.945030

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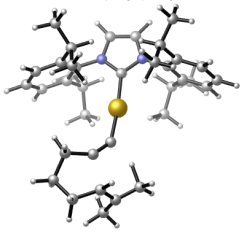

E = -1645.368049 h.
G = -1644.681099 h.

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6	0.199911	1.028572	0.424866
6	0.694213	-0.251670	1.014719
1	-0.089649	-1.022049	0.960710
1	0.926514	-0.100894	2.083744
79	-2.873802	1.578986	0.123532
6	1.966848	-0.652419	0.283077
1	2.460854	-1.518088	0.745027
1	1.715360	-0.928808	-0.753073
6	2.853045	0.593336	0.287908
1	3.364744	0.669239	1.258614
1	3.638085	0.528494	-0.478730
6	1.970979	1.722947	-2.432476
1	1.055275	1.167821	-2.705809
1	2.174969	2.418222	-3.258064
1	2.790152	0.992756	-2.394108
6	0.833438	3.521732	-1.110555
1	-0.171535	2.888112	-0.726619
1	0.941697	4.246136	-0.294275
1	0.599926	4.011304	-2.062836
6	1.973216	1.813743	0.090713
1	1.929429	2.483750	0.956458
6	1.773999	2.448193	-1.138465
6	-4.920448	1.302352	0.242737
6	-7.154137	1.573623	0.481479
1	-8.073101	2.137205	0.581915
6	-6.908699	0.241110	0.457399
1	-7.567544	-0.615513	0.526505
7	-5.925975	2.203233	0.343765
7	-5.538410	0.097256	0.311719
6	-4.840435	-1.155218	0.237787
6	-4.673646	-1.752777	-1.019321
6	-4.317613	-1.702043	1.418309
6	-3.969387	-2.957144	-1.070227
6	-3.609703	-2.900572	1.312092
6	-3.439278	-3.524549	0.082069
1	-3.825935	-3.449864	-2.032118
1	-3.184356	-3.349321	2.210026
1	-2.886795	-4.461083	0.020887
6	-5.727694	3.624464	0.358278
6	-5.785215	4.321785	-0.857191
6	-5.464671	4.245102	1.586652
6	-5.569205	5.699915	-0.814175
6	-5.262260	5.626816	1.576340
6	-5.312788	6.346633	0.389425
1	-5.591710	6.275050	-1.739026
1	-5.054429	6.142930	2.513746
1	-5.147005	7.422922	0.400925
6	-5.381266	3.473000	2.887262
1	-5.589064	2.412862	2.676309
6	-6.003359	3.616707	-2.179388
1	-6.407618	2.613398	-1.975118
6	-5.201274	-1.130766	-2.294918
1	-5.686908	-0.175179	-2.042372
6	-4.479066	-1.037807	2.769420
1	-5.099283	-0.137369	2.643251
6	-6.432719	3.956693	3.882672
1	-6.267429	5.006644	4.163460
1	-7.446409	3.875738	3.465532
1	-6.397108	3.358543	4.803434
6	-3.976830	3.554383	3.481756
1	-3.706199	4.591936	3.725488
1	-3.918465	2.968126	4.409510
1	-3.221859	3.163172	2.781902
6	-5.201158	-1.954650	3.753741
1	-6.175304	-2.278744	3.361648
1	-4.611202	-2.855557	3.974853
1	-5.374516	-1.434066	4.705477
6	-3.126367	-0.593385	3.323192
1	-3.250288	-0.114836	4.304778
1	-2.448649	-1.449901	3.452151
1	-2.635446	0.125753	2.647639
6	-6.250773	-2.023527	-2.952554
1	-5.819134	-2.989325	-3.252716
1	-7.091397	-2.227921	-2.274735
1	-6.652330	-1.544872	-3.856278
6	-4.062789	-0.823447	-3.265666
1	-3.567347	-1.744231	-3.605539
1	-4.448068	-0.306382	-4.155462
1	-3.298019	-0.183409	-2.802003
6	-7.007690	4.337043	-3.073775
1	-7.964118	4.505361	-2.560715
1	-6.630461	5.312048	-3.412939
1	-7.207777	3.738721	-3.972830
6	-4.667172	3.440576	-2.902241
1	-4.805124	2.893197	-3.845512
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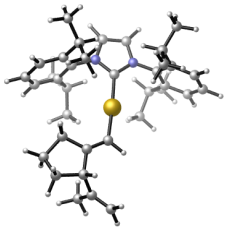
VIIIc



E = -1645.448646 h.
G = -1644.756535 h.

6	-0.814669	2.179600	0.005135
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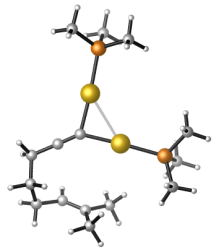
6	-0.069556	-0.264426	0.133202

1	-1.008220	-0.603352	-0.330463
1	-0.128258	-0.539425	1.202235
79	-2.831141	1.829098	0.212562
6	1.181540	-0.888405	-0.481077
1	1.376003	-1.910236	-0.129746
1	1.078199	-0.934150	-1.575778
6	2.287943	0.093207	-0.092103
1	2.590831	-0.099471	0.947938
1	3.191967	0.002243	-0.710426
6	1.667524	1.565885	-2.747577
1	0.608864	1.275193	-2.824098
1	1.903789	2.215944	-3.599258
1	2.256444	0.642863	-2.856610
6	2.438655	3.491785	-1.400528
1	-0.436032	3.207505	-0.108794
1	2.647922	3.991877	-0.453550
1	2.646591	4.057959	-2.309778
6	1.643624	1.495165	-0.170650
1	1.999733	2.119374	0.663673
6	1.950062	2.247960	-1.442903
6	-4.851900	1.350479	0.423279
6	-7.102277	1.394837	0.672626
1	-8.074726	1.861213	0.768609
6	-6.721674	0.094263	0.665860
1	-7.286630	-0.825352	0.754421
7	-5.945263	2.144508	0.518194
7	-5.344268	0.090727	0.513312
6	-4.516369	-1.080552	0.471711
6	-4.207599	-1.637583	-0.777054
6	-4.014831	-1.585309	1.680094
6	-3.375313	-2.759087	-0.789760
6	-3.183161	-2.704743	1.612683
6	-2.869647	-3.288740	0.391295
1	-3.113842	-3.220580	-1.742125
1	-2.770507	-3.120285	2.532226
1	-2.219669	-4.162135	0.359317
6	-5.888020	3.578834	0.505185
6	-6.008149	4.243793	-0.724128
6	-5.681122	4.245546	1.720173
6	-5.912560	5.636100	-0.710105
6	-5.600874	5.639230	1.681180
6	-5.711751	6.327133	0.479455
1	-5.990972	6.187679	-1.646588
1	-5.443958	6.191380	2.607782
1	-5.641052	7.413823	0.468545
6	-5.551870	3.513940	3.039810
1	-5.583668	2.431307	2.843803
6	-6.178869	3.494417	-2.029077
1	-6.496872	2.466772	-1.795692
6	-4.709665	-1.053682	-2.080501
1	-5.341287	-0.181716	-1.852860
6	-4.314243	-0.940345	3.017377
1	-5.030564	-0.120324	2.857061
6	-7.247256	4.111759	-2.926345
1	-8.204677	4.230930	-2.401601
1	-6.942392	5.098374	-3.302672
1	-7.417690	3.470979	-3.801897
6	-4.844511	3.408633	-2.771220
1	-4.959970	2.845560	-3.708234
1	-4.476811	4.413747	-3.026012
1	-4.071320	2.911980	-2.163602
6	-4.215056	3.810904	3.714183
1	-4.126022	4.872713	3.984919
1	-4.116499	3.224332	4.638192
1	-3.369995	3.557825	3.056990
6	-6.721000	3.852211	3.961938
1	-6.730517	4.922400	4.214491
1	-7.686035	3.610296	3.494675
1	-6.648447	3.289205	4.902545
6	-4.964280	-1.929991	3.980680
1	-5.882619	-2.358707	3.555352
1	-4.287971	-2.761034	4.226453
1	-5.228764	-1.430203	4.922490
6	-3.049906	-0.328655	3.618555
1	-3.274251	0.155081	4.579636
1	-2.282508	-1.095012	3.800946
1	-2.614939	0.429930	2.948092
6	-5.575768	-2.056724	-2.837806
1	-5.002449	-2.950600	-3.122305
1	-6.431423	-2.384897	-2.231098
1	-5.967802	-1.608092	-3.760842
6	-3.545628	-0.565212	-2.940865
1	-2.877426	-1.393750	-3.217013
1	-3.917290	-0.114691	-3.871598
1	-2.945020	0.190187	-2.410006

IVa

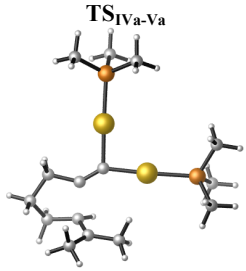


E = -1543.877505 h.
G = -1543.517617 h.

6	4.456298	0.822919	3.143394
1	4.846116	0.008336	2.514428
1	5.253956	1.581156	3.196250
6	4.196942	1.348247	5.645990
1	4.007094	0.854831	6.610947
1	5.220543	1.749189	5.706103
6	3.240260	2.484973	5.433616
1	3.642626	3.364665	4.920859
6	1.949074	2.520064	5.793074
6	1.227970	1.379707	6.442195
1	0.664931	1.714102	7.326697
1	0.485293	0.957436	5.743658
1	1.891322	0.561946	6.747692
6	1.095207	3.715509	5.509155
1	0.239604	3.433741	4.870096
1	0.666796	4.132132	6.434517
1	1.649334	4.512708	4.994959
79	1.918633	1.804278	-0.220671
15	1.667058	1.814001	-2.541235
6	2.705690	0.601749	-3.415941
1	2.461990	-0.411661	-3.075703
1	2.532908	0.670212	-4.498585
1	3.763872	0.797148	-3.205417
6	2.081061	3.409606	-3.313263
1	1.939171	3.352656	-4.401070
1	1.435916	4.196973	-2.905652
1	3.124895	3.667234	-3.097554
6	-0.023825	1.456651	-3.114044
1	-0.722448	2.198021	-2.707489
1	-0.060922	1.487182	-4.211426
1	-0.331416	0.461787	-2.770410
6	4.166289	0.277563	4.553757
1	3.190819	-0.232261	4.552691
1	4.924071	-0.484183	4.782605

6	3.284985	1.363436	2.472750
6	2.274349	1.765080	1.882826
79	0.337913	2.521488	2.205775
15	-1.818829	3.318261	2.655151
6	-2.610927	2.555782	4.107497
1	-2.030159	2.779738	5.011177
1	-3.628825	2.950447	4.229316
1	-2.656532	1.467467	3.981586
6	-1.905969	5.107081	2.985863
1	-1.565749	5.665646	2.105575
1	-2.939948	5.394826	3.219839
1	-1.259404	5.363927	3.834041
6	-3.006853	3.048399	1.300153
1	-3.095255	1.975237	1.092812
1	-3.992682	3.445408	1.577983
1	-2.656029	3.553232	0.391830

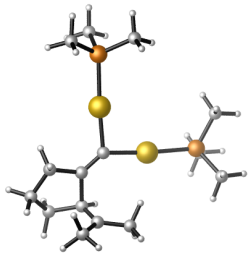
$TS_{IVa\text{-}Va}$



E = -1543.841247 h.
G = -1543.482122 h.

6	4.182279	1.185790	2.916185
1	4.029983	0.245625	2.369715
1	4.757605	1.849923	2.251658
6	4.567326	2.190477	5.075640
1	4.841824	2.050999	6.130444
1	5.107721	3.077247	4.716966
6	3.078293	2.452095	4.927707
1	2.797285	3.501665	4.811766
6	2.128569	1.684836	5.609583
6	2.394821	0.305795	6.098747
1	1.671667	0.015287	6.868786
1	2.295570	-0.421256	5.275702
1	3.407380	0.192170	6.506592
6	0.757669	2.203072	5.728778
1	0.242991	2.039849	4.747088
1	0.167802	1.687970	6.494723
1	0.728105	3.286622	5.893090
79	1.804273	1.859294	0.354202
15	1.726847	1.560753	-1.981028
6	2.739624	0.188907	-2.623856
1	2.425453	-0.755571	-2.163544
1	2.628712	0.114024	-3.714097
1	3.795386	0.359610	-2.380848
6	2.284119	3.003188	-2.947651
1	2.219200	2.789550	-4.023352
1	1.658647	3.873156	-2.713576
1	3.322797	3.244517	-2.691228
6	0.058204	1.213162	-2.630075
1	-0.615771	2.042236	-2.381571
1	0.089242	1.087066	-3.720976
1	-0.334917	0.297235	-2.172424
6	4.936104	0.989205	4.217491
1	4.624363	0.055991	4.703613
1	6.018488	0.919992	4.054291
6	2.845530	1.854382	3.157818
6	1.812884	2.158241	2.442076
79	-0.080782	2.985733	2.523843
15	-2.250184	3.918628	2.505237
6	-3.352192	3.219108	3.779481
1	-2.909872	3.365663	4.773288
1	-4.335834	3.706733	3.746387
1	-3.478399	2.142423	3.612336
6	-2.300804	5.713582	2.824461
1	-1.744931	6.245595	2.042930
1	-3.339487	6.070352	2.835362
1	-1.834683	5.932222	3.792840
6	-3.190830	3.726262	0.954307
1	-3.294356	2.662005	0.710163
1	-4.190119	4.171500	1.055129
1	-2.656392	4.221153	0.134192

Va

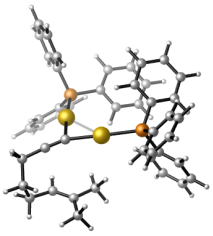


E = -1543.842820 h.
G = -1543.482514 h.

6	4.069541	1.103200	3.038204
1	3.886872	0.035670	2.843607
1	4.504109	1.509547	2.114722
6	4.403773	2.479176	5.023913
1	4.669047	2.451484	6.089516
1	4.767825	3.435098	4.624266
6	2.892015	2.452492	4.822780
1	2.425157	3.441302	4.833302
6	2.085936	1.471864	5.474263
6	2.589643	0.129168	5.852454
1	1.837662	-0.434701	6.412577
1	2.862037	-0.467013	4.968487
1	3.499673	0.211363	6.464448
6	0.677360	1.802504	5.720337
1	0.186291	2.008466	4.736407
1	0.122998	1.010309	6.232258
1	0.583280	2.749297	6.270839
79	1.816082	1.816113	0.385151
15	1.727547	1.492157	-1.959380
6	2.729794	0.108193	-2.595197
1	2.413883	-0.829790	-2.122723
1	2.612942	0.021284	-3.683940
1	3.787768	0.275702	-2.359333
6	2.288568	2.919371	-2.948075
1	2.218468	2.694237	-4.021134
1	1.668925	3.795602	-2.721753
1	3.329470	3.158478	-2.698368
6	0.055626	1.145244	-2.603629
1	-0.615695	1.977658	-2.358897
1	0.082439	1.010451	-3.693621
1	-0.339068	0.233934	-2.137929
6	5.003078	1.318106	4.231390
1	5.066022	0.413649	4.848534
1	6.027174	1.546027	3.912163
6	2.763795	1.851802	3.277125
6	1.777357	2.137817	2.446272
79	-0.086098	3.026103	2.560185
15	-2.226708	4.048252	2.516792

6	-3.376270	3.395874	3.774955
1	-2.944072	3.523837	4.775513
1	-4.338439	3.923718	3.727677
1	-3.544716	2.325306	3.605300
6	-2.219462	5.845937	2.830811
1	-1.633124	6.356532	2.057343
1	-3.245473	6.237933	2.823412
1	-1.761867	6.051807	3.806098
6	-3.159316	3.889354	0.956187
1	-3.308541	2.829432	0.716842
1	-4.138937	4.378577	1.046059
1	-2.597163	4.356140	0.138181

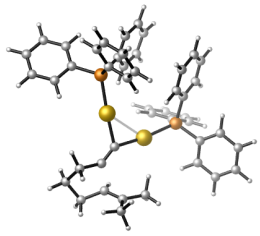
IVb



E = -2693.398520 h.
G = -2692.745564 h.

6	4.139881	0.783913	3.648460
1	4.449459	-0.203898	3.277732
1	4.907201	1.502516	3.320317
6	3.805638	2.140252	5.793315
1	4.591792	2.837875	5.466063
1	2.858980	2.531972	5.387574
6	3.716827	2.074421	7.287474
1	2.747414	1.757096	7.685515
6	4.700756	2.302660	8.168679
6	6.096243	2.702201	7.798030
1	6.370709	3.654110	8.278288
1	6.818863	1.957620	8.166413
1	6.251726	2.811152	6.718566
6	4.472090	2.161106	9.642996
1	5.156681	1.417579	10.080044
1	4.675111	3.107668	10.168002
1	3.443589	1.857924	9.876750
79	1.863847	1.692924	0.470856
15	1.874772	2.006019	-1.840053
6	4.080911	0.767463	5.183332
1	3.315462	0.048737	5.513121
1	5.046205	0.392480	5.554779
6	2.857755	1.145392	3.064167
6	1.744311	1.454783	2.621633
79	-0.276000	1.937952	2.528820
15	-2.567746	2.456903	2.433302
6	1.985427	0.456498	-2.788687
6	1.249955	-0.645295	-2.336228
6	2.742767	0.353422	-3.958278
6	1.264934	-1.835422	-3.053699
1	0.668670	-0.569575	-1.414967
6	2.760607	-0.844081	-4.668539
1	3.318550	1.206209	-4.317959
6	2.021958	-1.935012	-4.219688
1	0.690931	-2.689705	-2.699303
1	3.353308	-0.921401	-5.578213
1	2.038900	-2.869272	-4.778158
6	0.332672	2.814628	-2.369612
6	-0.201905	2.618997	-3.646969
6	-0.312907	3.671033	-1.470329
6	-1.368455	3.280084	-4.019202
1	0.292888	1.952341	-4.353799
6	-1.477610	4.330724	-1.846661
1	0.096183	3.805487	-0.465506
6	-2.004951	4.134083	-3.120875
1	-1.783785	3.125966	-5.013570
1	-1.984527	4.984005	-1.136917
1	-2.922970	4.642872	-3.411033
6	3.247549	3.057382	-2.406253
6	4.505097	2.856122	-1.825659
6	3.086434	4.026335	-3.399580
6	5.592798	3.616009	-2.238498
1	4.627052	2.100997	-1.046483
6	4.178079	4.790512	-3.803469
1	2.111035	4.187615	-3.858728
6	5.427469	4.586637	-3.224921
1	6.569088	3.457825	-1.783646
1	4.049696	5.548903	-4.573750
1	6.277443	5.189113	-3.540736
6	-3.249783	2.199196	0.765056
6	-2.590148	1.323794	-0.104641
6	-4.412807	2.851209	0.340483
6	-3.090321	1.099190	-1.383496
1	-1.673348	0.826851	0.222208
6	-4.912528	2.619710	-0.937042
1	-4.929844	3.541934	1.007689
6	-4.251444	1.745832	-1.798023
1	-2.560271	0.434391	-2.064640
1	-5.817838	3.128854	-1.262775
1	-4.637021	1.578861	-2.802622
6	-3.552938	1.445709	3.581536
6	-4.737648	0.811696	3.203077
6	-3.085432	1.323038	4.895994
6	-5.449047	0.059846	4.135580
1	-5.109895	0.900838	2.182690
6	-3.804159	0.579755	5.824063
1	-2.156716	1.816349	5.190338
6	-4.985071	-0.054997	5.442263
1	-6.370172	-0.437491	3.837077
1	-3.438514	0.489266	6.845288
1	-5.543863	-0.643676	6.167704
6	-2.931669	4.190526	2.855827
6	-2.046374	5.176682	2.406303
6	-4.073047	4.557312	3.573691
6	-2.307491	6.518076	2.661510
1	-1.145640	4.888742	1.859985
6	-4.325733	5.901306	3.833852
1	-4.766440	3.795661	3.931299
6	-3.446548	6.879689	3.377871
1	-1.615850	7.281144	2.308978
1	-5.213311	6.183312	4.397496
1	-3.647263	7.929346	3.585711

$TS_{IVb\text{-}Vb}$



E = -2693.373288 h.
G = -2692.713543 h.

6	2.721969	1.448697	5.605094
1	3.142968	2.311331	6.147695
1	1.660922	1.378798	5.876511
6	4.862547	0.405333	5.251686

1	5.508574	1.010648	5.900887
1	5.388625	-0.541103	5.074240
6	4.643059	1.114511	3.926481
1	4.558945	0.455990	3.057684
6	5.173212	2.372705	3.647302
6	5.495946	3.389718	4.678706
1	4.940465	4.316801	4.467315
1	5.282171	3.079500	5.705459
1	6.561443	3.657592	4.610899
6	5.311255	2.789399	2.241518
1	4.285396	2.899941	1.809091
1	5.829286	3.748534	2.126190
1	5.801334	2.021108	1.630448
79	2.103282	2.220834	1.056002
15	1.840747	2.595480	-1.266033
6	3.511473	0.193218	5.929881
1	3.615292	0.024526	7.008707
1	2.998490	-0.680357	5.501194
6	2.829874	1.658811	4.123454
6	2.076485	1.899332	3.102196
79	-0.022659	1.968916	3.199104
15	-2.381668	2.059104	3.143057
6	1.920645	1.068022	-2.257711
6	1.407210	-0.106817	-1.696494
6	2.435411	1.046430	-3.557257
6	1.397403	-1.286672	-2.432570
1	1.020491	-0.094727	-0.675122
6	2.429704	-0.138133	-4.287782
1	2.840308	1.956755	-4.000790
6	1.909685	-1.302346	-3.728037
1	0.997479	-2.197963	-1.991129
1	2.832977	-0.150566	-5.298804
1	1.908113	-2.227383	-4.302074
6	0.219525	3.339503	-1.639812
6	-0.381151	3.213293	-2.896683
6	-0.434386	4.053267	-0.629297
6	-1.623345	3.792246	-3.135786
1	0.121203	2.661773	-3.692149
6	-1.671695	4.641379	-0.875895
1	0.030102	4.145236	0.356300
6	-2.270339	4.500456	-2.125307
1	-2.089824	3.685730	-4.113761
1	-2.176322	5.196615	-0.086250
1	-3.245730	4.947243	-2.312340
6	3.106228	3.704894	-1.967869
6	4.448344	3.389581	-1.718948
6	2.789929	4.847952	-2.703872
6	5.460272	4.209265	-2.202253
1	4.698228	2.492539	-1.147992
6	3.808539	5.671241	-3.180278
1	1.749653	5.102367	-2.905810
6	5.139683	5.354466	-2.930418
1	6.501342	3.958057	-2.006447
1	3.556540	6.563137	-3.751495
1	5.931987	6.001784	-3.302441
6	-3.010891	1.792084	1.452850
6	-2.238126	1.022041	0.575625
6	-4.221180	2.336058	1.012023
6	-2.672104	0.796447	-0.727035
1	-1.287047	0.607968	0.919586
6	-4.650647	2.111721	-0.292607
1	-4.829274	2.940308	1.685880
6	-3.874559	1.348774	-1.162714
1	-2.060772	0.204622	-1.407882
1	-5.591696	2.539944	-0.633746
1	-4.206793	1.185479	-2.186781
6	-3.187692	0.825657	4.213427
6	-4.313907	0.099909	3.818680
6	-2.649986	0.632676	5.491639
6	-4.897104	-0.808660	4.698514
1	-4.739410	0.239764	2.824690
6	-3.240499	-0.269085	6.368917
1	-1.763680	1.194161	5.795440
6	-4.364001	-0.991597	5.971058
1	-5.772946	-1.375402	4.387359
1	-2.818646	-0.413623	7.362039
1	-4.821731	-1.703435	6.655842
6	-3.045190	3.674244	3.665986
6	-2.304715	4.819674	3.351409
6	-4.264877	3.799993	4.336504
6	-2.785169	6.078587	3.695043
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6	-4.001873	6.198755	4.362842
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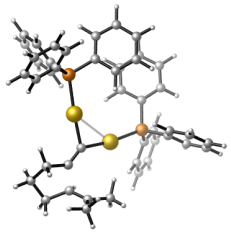
Vb



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1	5.227371	3.615195	5.207412
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1	2.920869	3.744683	4.658083
6	2.482712	1.889169	5.535311
6	2.856207	0.528522	5.978604
1	2.786030	0.484555	7.076659
1	2.115747	-0.197648	5.608261
1	3.856612	0.203366	5.682055
6	1.126953	2.347404	5.849881
1	0.577170	2.477343	4.882345
1	0.563054	1.650747	6.479092
1	1.135358	3.349685	6.298899
79	1.817622	1.840395	0.436241
15	1.511266	1.437893	-1.882289
6	5.387807	2.235059	3.503743
1	6.378421	1.770803	3.581282
1	5.477361	3.111865	2.845578
6	3.010347	1.997233	3.226705
6	1.954110	2.239630	2.482479
79	0.074289	3.084578	2.634235
15	-2.111181	4.006173	2.482599
6	2.275888	-0.120175	-2.442582
6	3.622145	-0.331984	-2.116955
6	1.577024	-1.094677	-3.157289
6	4.261747	-1.499259	-2.514771
1	4.170312	0.426237	-1.553382
6	2.220236	-2.268226	-3.545053
1	0.529292	-0.941608	-3.414977

6	3.559393	-2.470361	-3.227387
1	5.309251	-1.655802	-2.263012
1	1.669744	-3.026282	-4.099573
1	4.059421	-3.387991	-3.532462
6	2.215422	2.737064	-2.951697
6	2.212258	4.052926	-2.475120
6	2.720015	2.465393	-4.227065
6	2.690044	5.087601	-3.272753
1	1.840101	4.263941	-1.470260
6	3.203072	3.502777	-5.019252
1	2.736554	1.442649	-4.604476
6	3.186079	4.811860	-4.544712
1	2.684348	6.109059	-2.896511
1	3.595895	3.286518	-6.011266
1	3.565853	5.620368	-5.167061
6	-0.252865	1.336996	-2.330050
6	-1.182271	1.070305	-1.318600
6	-0.695197	1.506981	-3.646495
6	-2.536033	0.960242	-1.620939
1	-0.838361	0.957461	-0.287489
6	-2.049797	1.400411	-3.944839
1	0.020425	1.720851	-4.441522
6	-2.969126	1.127195	-2.933460
1	-3.253128	0.750543	-0.828379
1	-2.389271	1.533168	-4.970731
1	-4.029633	1.052722	-3.169634
6	-2.274718	5.651311	3.247677
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6	-1.606496	7.161202	5.015138
1	-0.791805	5.183204	4.746581
6	-3.273940	7.844641	3.409209
1	-3.777997	6.406426	1.888634
6	-2.495902	8.117664	4.531597
1	-0.995711	7.376074	5.890297
1	-3.968409	8.592121	3.029533
1	-2.581835	9.082041	5.029503
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6	-1.645950	4.450777	-0.213769
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6	-1.992774	4.611343	-1.551139
1	-0.598451	4.515925	0.091988
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1	-4.747696	3.898981	1.090436
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6	-4.406920	3.469609	4.059916
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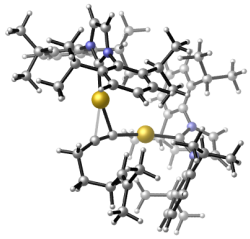
IVc



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6	1.355181	-3.545041	0.458402
1	1.170259	-4.592153	0.734658
1	0.531197	-3.261471	-0.218748
6	2.654629	-3.401026	-0.275133
1	2.760869	-2.483643	-0.870214
6	3.691835	-4.252356	-0.272741
6	3.731498	-5.547488	0.479391
1	3.893772	-6.390598	-0.210981
1	4.581300	-5.561944	1.179248
1	2.822628	-5.752993	1.056209
6	4.932664	-3.968286	-1.063767
1	5.816975	-3.909218	-0.409734
1	5.139331	-4.779249	-1.780488
1	4.860036	-3.026801	-1.624140
6	2.525206	2.949841	-1.245359
7	2.073119	4.221985	-1.213392
7	3.737030	3.021671	-1.839575
6	4.045884	4.328159	-2.176269
1	4.984553	4.586146	-2.650596
6	2.994147	5.087456	-1.778988
1	2.809329	6.152760	-1.835771
6	0.822246	4.621734	-0.631404
6	-0.323213	4.629130	-1.439738
6	-1.519896	5.033662	-0.844901
6	-0.410053	5.376616	1.269477
6	-1.561351	5.409736	0.492727
1	-2.434393	5.046982	-1.438015
1	-0.459013	5.663293	2.319846
1	-2.504122	5.727595	0.935592
6	4.594569	1.884455	-2.023072
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6	5.564985	1.629680	-1.044949
6	5.232622	-0.043532	-3.278374
6	6.381483	0.512092	-1.230177
6	6.220790	-0.312139	-2.336959
1	5.112808	-0.704042	-4.137272
1	7.150950	0.284497	-0.492622
1	6.869627	-1.177306	-2.465956
6	-0.302495	4.155930	-2.877733
1	0.746613	4.015552	-3.183321
1	5.023571	3.339791	0.116534
6	5.721211	2.492109	0.190245
6	3.339955	1.365768	-4.186486
1	2.636433	2.104611	-3.769242
6	1.256012	-2.695105	1.729941
1	1.961106	-3.077788	2.483224
1	0.245449	-2.800164	2.150777
6	0.811687	4.975131	0.725039
6	2.047834	4.912752	1.597396
1	2.898993	4.584223	0.981135

6	0.239035	-0.579655	-0.726934
79	1.546205	1.239949	-0.706209
79	-0.547710	-0.993020	-2.559330
6	-1.249504	-1.717128	-4.360172
6	-2.285842	-2.084797	-6.332588
1	-2.875638	-1.818892	-7.201130
6	-1.702330	-3.247923	-5.960548
1	-1.684944	-4.226314	-6.423787
7	-1.996152	-1.156507	-5.340939
7	-1.070534	-3.003756	-4.751948
6	-0.523277	-4.028741	-3.900883
6	0.846036	-4.325715	-3.970927
6	-1.403852	-4.672494	-3.018258
6	1.327242	-5.321069	-3.117073
6	-0.871960	-5.661123	-2.188044
6	0.477815	-5.983528	-2.237737
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1	-1.527640	-6.179075	-1.488353
1	0.874046	-6.757174	-1.581003
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1	-0.802863	4.818976	-4.874548
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1	3.224229	2.223946	-6.181551
6	2.527475	0.127610	-4.553984
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1	2.145297	-0.390020	-3.659272
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1	7.206240	3.737718	1.162719
6	5.348779	1.709426	1.447999
1	6.011754	0.844228	1.591472
1	5.437038	2.348258	2.337562
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6	3.151992	-3.376571	-4.407639
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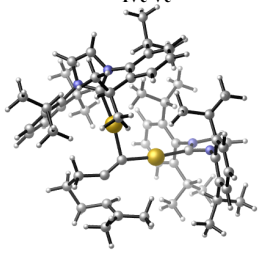

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6	-0.702433	-3.528550	0.638740
1	-0.367211	-3.119361	-0.340511
1	-0.003343	-4.311221	0.955823
1	-1.686113	-3.981820	0.447337
6	2.641093	2.767768	-1.880808

7	2.315094	3.981683	-1.360335
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1	4.933126	4.733208	-3.158282
6	3.186943	4.966295	-1.798063
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6	1.377658	4.170166	-0.282455
6	0.022656	4.391350	-0.571797
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6	0.976014	4.325829	2.072126
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6	5.458144	1.289937	-2.478828
6	5.495882	1.089857	-5.280446
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6	6.387592	0.351192	-4.513825
1	5.523483	1.007526	-6.366598
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1	7.110086	-0.302934	-5.000133
6	-0.489358	4.456099	-1.993977
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6	5.509042	1.427592	-0.971195
6	3.583054	2.713121	-5.537653
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6	3.334422	3.827283	1.343862
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6	2.671100	-3.893876	-4.371903
6	1.013145	-5.395465	-3.324222
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6	-3.574804	-1.694625	-4.189226
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1	-5.552900	-1.144059	-3.549302
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6	-0.851937	0.695895	-5.513408
1	-0.092940	-0.095386	-5.403008
6	-3.765540	-3.162489	-3.866049
1	-2.848531	-3.707251	-4.138240
6	-0.430164	-5.749296	-3.019613
1	-1.003114	-4.807976	-2.989203
6	2.994589	-2.601693	-5.091004
1	2.109769	-2.292614	-5.670397
6	3.990188	5.000143	2.067908
1	3.906425	5.929935	1.488569
1	3.528655	5.173613	3.050533
1	5.057577	4.798308	2.233815
6	3.478770	2.537684	2.150517
1	4.539225	2.328522	2.352093
1	2.969102	2.612859	3.122360
1	3.054446	1.674615	1.616108
6	6.748538	2.213307	-0.547637
1	7.670843	1.673783	-0.809002
1	6.787652	3.198499	-1.034199
1	6.752366	2.373683	0.540079
6	5.439651	0.078844	-0.262004
1	6.309651	-0.553171	-0.489354
1	5.420432	0.228251	0.826872
1	4.531744	-0.475520	-0.542664
6	4.281746	3.867237	-6.253626
1	4.768807	4.550727	-5.544706
1	5.053417	3.493136	-6.942353
1	3.561274	4.449282	-6.844524
6	2.869347	1.811285	-6.542356
1	2.096218	2.380233	-7.078595
1	3.561309	1.412561	-7.297889
1	2.383136	0.957000	-6.045935
6	-0.476646	5.901701	-2.491210
1	-1.152813	6.524794	-1.886786
1	0.527295	6.344442	-2.431592
1	-0.810474	5.954766	-3.536964
6	-1.879306	3.850469	-2.151187
1	-2.647115	4.443499	-1.634953
1	-2.158024	3.824380	-3.213511
1	-1.924435	2.821532	-1.763193
6	4.159555	-2.719185	-6.066638
1	4.284568	-1.773053	-6.612509
1	5.109563	-2.919452	-5.551514
1	4.000552	-3.516694	-6.805094
6	3.272728	-1.514239	-4.052687
1	2.429331	-1.396321	-3.354381
1	4.167523	-1.762225	-3.460572
1	3.448648	-0.545247	-4.541068
6	-0.978592	1.021645	-7.000413
1	-1.729894	1.807968	-7.166983
1	-0.020955	1.382166	-7.402136
1	-1.281010	0.142173	-7.585948
6	-0.353555	1.906126	-4.728272
1	-0.348708	1.704257	-3.646091
1	0.674982	2.155766	-5.025870
1	-0.972306	2.797432	-4.910927
6	-1.034572	-6.625779	-4.117054
1	-0.986831	-6.148752	-5.104835
1	-0.501509	-7.586359	-4.179613
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6	-0.603873	-6.427358	-1.665132
1	-1.670918	-6.478755	-1.408958
1	-0.225981	-7.459519	-1.673325
1	-0.086101	-5.884370	-0.863086
6	-4.910628	-3.768894	-4.671715
1	-5.872324	-3.299171	-4.420225
1	-4.749382	-3.646901	-5.751969
1	-4.999850	-4.843761	-4.461401
6	-3.975240	-3.365501	-2.367117
1	-4.911474	-2.900830	-2.025186
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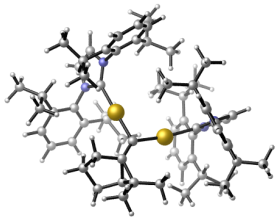
1	-3.149740	-2.922651	-1.789667

Vc



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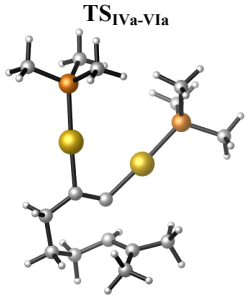
1	2.409779	-0.138883	1.448239
6	-0.831660	-0.439587	2.397273
1	-0.950026	-1.021403	3.322877
1	-1.696884	0.229198	2.318112
6	-0.766379	-1.364895	1.201231
1	-1.485490	-1.214274	0.396092
6	-0.045148	-2.643218	1.216325
6	0.364140	-3.297007	2.519500
1	-0.405640	-4.028353	2.801427
1	1.308522	-3.844611	2.396178
1	0.478802	-2.610916	3.362537
6	-0.438227	-3.683753	0.193981
1	-0.868818	-3.245344	-0.713044
1	0.426486	-4.296585	-0.104981
1	-1.191359	-4.355193	0.631313
6	2.604697	2.628075	-1.783334
7	2.085307	3.832333	-1.432651
7	3.616302	2.924733	-2.635736
6	3.723931	4.298317	-2.819286
1	4.480649	4.725725	-3.464935
6	2.755964	4.868575	-2.065547
1	2.484058	5.904173	-1.903789
6	1.152858	4.040908	-0.354371
6	-0.225108	3.926450	-0.584006
6	-1.081204	4.193692	0.487238
6	0.788011	4.624205	1.940967
6	-0.583711	4.550143	1.733757
1	-2.158133	4.123253	0.335111
1	1.170731	4.883457	2.928147
1	-1.269718	4.762498	2.552354
6	4.586349	1.992209	-3.147064
6	4.559960	1.657647	-4.508804
6	5.577632	1.516060	-2.268925
6	5.592068	0.850988	-4.996563
6	6.568897	0.691865	-2.804556
6	6.587321	0.372531	-4.156186
1	5.610814	0.590400	-6.054820
1	7.354742	0.313319	-2.151647
1	7.380598	-0.257640	-4.555553
6	-0.807349	3.506279	-1.914260
1	0.022736	3.290167	-2.602875
1	4.695861	2.384223	-0.525606
6	5.644142	1.905645	-0.806061
6	3.468061	2.114155	-5.452437
1	2.709678	2.664299	-4.873788
6	0.494529	0.333509	2.405641
1	0.742218	0.760763	3.386328
1	0.408189	1.163053	1.684179
6	1.687420	4.365264	0.904940
6	3.177129	4.394775	1.185032
1	3.718693	4.189724	0.249741
6	0.872727	-0.933130	-0.578792
79	1.848011	0.795536	-1.130334
79	0.072549	-1.567598	-2.358546
6	-0.471084	-2.170553	-4.278917
6	-1.342545	-2.354645	-6.357175
1	-1.996633	-2.090305	-7.178804
6	-0.399722	-3.317312	-6.227692
1	-0.051938	-4.082500	-6.910430
7	-1.370143	-1.659905	-5.153852
7	0.117058	-3.195060	-4.946936
6	0.965771	-4.174922	-4.320508
6	2.330560	-3.907717	-4.146808
6	0.361474	-5.364845	-3.879284
6	3.103168	-4.885817	-3.516393
6	1.180891	-6.311150	-3.260806
6	2.537743	-6.076089	-3.079110
1	4.168294	-4.706948	-3.370172
1	0.745451	-7.246610	-2.909968
1	3.158945	-6.826796	-2.592881
6	-2.368001	-0.673035	-4.840782
6	-2.240550	0.617843	-5.370115
6	-3.470459	-1.069973	-4.063103
6	-3.279390	1.520663	-5.128953
6	-4.471829	-0.123388	-3.837929
6	-4.385999	1.155311	-4.375006
1	-3.210408	2.530365	-5.534081
1	-5.344112	-0.399478	-3.245557
1	-5.185071	1.873932	-4.199576
6	-1.016259	1.077417	-6.131703
1	-0.329371	0.224685	-6.241887
6	-3.624907	-2.470255	-3.507219
1	-2.681121	-3.012560	-3.655787
6	-1.120045	-5.653810	-4.031357
1	-1.602165	-4.805409	-4.540159
6	2.984624	-2.621099	-4.598021
1	2.205475	-1.961611	-5.009380
6	3.558231	3.295375	2.175730
1	4.642639	3.297500	2.355417
1	3.063663	3.440131	3.147171
1	3.272424	2.300249	1.802710
6	3.635670	5.763526	1.680282
1	3.376119	6.558071	0.967136
1	3.178399	6.017237	2.647020
1	4.725883	5.773066	1.817318
6	-1.639823	4.626189	-2.532147
1	-2.492776	4.892401	-1.891263
1	-1.040006	5.533597	-2.688432
1	-2.043226	4.313798	-3.505886
6	-1.632487	2.227179	-1.765712
1	-2.541839	2.404636	-1.172623
1	-1.948948	1.855564	-2.751817
1	-1.054410	1.429814	-1.270384
6	6.754182	2.930117	-0.577954
1	7.741694	2.506693	-0.813218
1	6.613946	3.822462	-1.204494
1	6.771497	3.255405	0.472092
6	5.810942	0.693999	0.106065
1	6.771201	0.183453	-0.053385
1	5.782707	1.005721	1.159698
1	5.006430	-0.040008	-0.052969
6	4.013717	3.057762	-6.521768
1	4.511547	3.932074	-6.080684
1	4.743973	2.546847	-7.165969
1	3.198670	3.419593	-7.164299
6	2.772363	0.915928	-6.096638

1	1.998772	1.254227	-6.800112
1	3.476156	0.294413	-6.668303
1	2.291134	0.279488	-5.338014
6	3.636272	-1.888387	-3.425464
1	3.980200	-0.894568	-3.746092
1	2.928687	-1.749957	-2.592806
1	4.511530	-2.435057	-3.042930
6	4.002112	-2.886102	-5.705189
1	4.794848	-3.565844	-5.360787
1	3.529714	-3.340262	-6.587501
1	4.485067	-1.949420	-6.018434
6	-1.368844	1.572510	-7.531405
1	-2.003136	2.469620	-7.496319
1	-0.457228	1.835800	-8.085935
1	-1.904703	0.805370	-8.107311
6	-0.288664	2.156184	-5.330380
1	0.071848	1.756649	-4.368742
1	0.577799	2.538448	-5.887669
1	-0.950689	3.009587	-5.121891
6	-4.706930	-3.237442	-4.264195
1	-5.693605	-2.766805	-4.144104
1	-4.483005	-3.281823	-5.339727
1	-4.782776	-4.268680	-3.891382
6	-3.889987	-2.454473	-2.004834
1	-4.862819	-2.003435	-1.763337
1	-3.894589	-3.479002	-1.606429
1	-3.111532	-1.883798	-1.474660
6	-1.354394	-6.891634	-4.894531
1	-0.883392	-6.789396	-5.882002
1	-0.947118	-7.795682	-4.419874
1	-2.430098	-7.053790	-5.047907
6	-1.792996	-5.801441	-2.668517
1	-2.859137	-6.039770	-2.790824
1	-1.339297	-6.611410	-2.079502
1	-1.714722	-4.873791	-2.083523

$TS_{IVa\text{-}VIa}$



E = -1543.840714 h.
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1	5.258247	1.618695	2.424705
6	4.347501	2.163095	5.109525
1	4.667951	2.128745	6.162348
1	4.885648	3.008062	4.654065
6	2.866105	2.480819	5.069058
1	2.632589	3.543882	4.966707
6	1.902215	1.742192	5.730938
6	2.106767	0.354394	6.229734
1	1.378702	0.118418	7.015526
1	1.943887	-0.372597	5.417723
1	3.116005	0.189913	6.625528
6	0.537783	2.290687	5.921186
1	-0.220373	1.598825	5.516223
1	0.330096	2.373982	6.999536
1	0.404389	3.279310	5.465144
79	2.441820	1.568056	0.577090
15	1.527146	1.748794	-1.586409
6	2.589035	1.327683	-3.005276
1	2.894276	0.276354	-2.942586
1	2.046071	1.489482	-3.946432
1	3.490623	1.951654	-2.997731
6	0.968889	3.450049	-1.935000
1	0.444153	3.500360	-2.898934
1	0.295727	3.787474	-1.135389
1	1.833388	4.124884	-1.957603
6	0.032809	0.733668	-1.834222
1	-0.702697	0.959369	-1.051424
1	-0.411052	0.934272	-2.818951
1	0.291877	-0.329885	-1.766374
6	4.781757	0.882870	4.401908
1	4.264652	0.011595	4.824468
1	5.854053	0.721832	4.578623
6	3.160104	1.473988	2.573486
6	2.205709	2.042755	3.277986
79	0.368553	2.809967	2.671373
15	-1.702805	3.674533	1.963831
6	-2.995111	3.492724	3.235799
1	-2.678970	3.998076	4.157322
1	-3.941546	3.930413	2.890241
1	-3.149195	2.429765	3.458844
6	-1.713502	5.456788	1.580966
1	-1.011198	5.671479	0.766269
1	-2.721917	5.774914	1.283031
1	-1.402064	6.026821	2.464881
6	-2.431247	2.899558	0.482554
1	-2.556535	1.822876	0.649823
1	-3.410994	3.346608	0.264764
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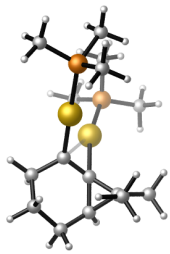
VIa



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6	3.866844	1.930908	5.391209
1	4.213985	0.971594	5.805234
1	4.170182	2.700999	6.114457
6	2.345487	1.977300	5.304023
1	1.846281	2.529487	6.103584
6	1.421703	0.878817	4.705638
6	1.984436	-0.456656	4.291114
1	1.349485	-0.922689	3.522653
1	2.996835	-0.370222	3.874412
1	2.021258	-1.144593	5.148917
6	0.041719	0.805382	5.311624
1	-0.678069	0.403145	4.582406
1	0.031375	0.144112	6.190003
1	-0.318023	1.794902	5.625635
79	2.085983	1.640134	0.917406
15	1.586237	0.732108	-1.214515
6	2.723638	1.223132	-2.552829

1	3.750544	0.938373	-2.293514
1	2.439709	0.729814	-3.492367
1	2.690307	2.310351	-2.692481
6	-0.064187	1.157612	-1.865163
1	-0.220806	0.688554	-2.846217
1	-0.837270	0.806647	-1.170545
1	-0.156441	2.245790	-1.969297
6	1.613913	-1.090958	-1.267176
1	0.887148	-1.496205	-0.552464
1	1.365228	-1.446433	-2.276331
1	2.610823	-1.455611	-0.991527
6	4.579140	2.212659	4.055172
1	4.732079	1.276187	3.494574
1	5.580164	2.622192	4.248034
6	2.522416	2.409633	2.804374
6	1.812703	2.072459	3.936132
79	0.443948	3.539418	2.909623
15	-1.344238	4.899438	2.232541
6	-2.893798	4.638332	3.151075
1	-2.738113	4.855152	4.214474
1	-3.678161	5.299074	2.757583
1	-3.215814	3.594978	3.050510
6	-1.036308	6.689206	2.348164
1	-0.162746	6.957658	1.742469
1	-1.912448	7.245190	1.987915
1	-0.835838	6.964901	3.390278
6	-1.788421	4.616162	0.489440
1	-2.047692	3.560266	0.342366
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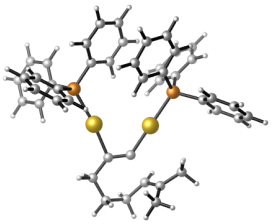
1	-0.931460	4.856998	-0.151908

$TS_{IVb\text{-}VIb}$



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G = -2692.711255 h.

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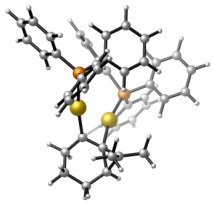
6	4.564983	1.118336	5.350907
1	5.591559	1.197300	5.740279
1	4.288461	0.056568	5.433448
6	4.581350	1.481675	3.878936
1	4.641790	0.626815	3.200290
6	5.150428	2.643565	3.386898
6	5.422544	3.849511	4.213043
1	6.222834	4.450480	3.764009
1	4.527124	4.492334	4.245687
1	5.696718	3.607826	5.246252
6	5.440981	2.778643	1.940295
1	4.899826	3.641331	1.512369
1	6.512232	2.992403	1.802154
1	5.189103	1.879647	1.365566
79	2.319412	2.184331	1.330460
15	1.835731	2.456812	-0.966321
6	3.619898	1.927945	6.232217
1	3.854368	2.999776	6.170455
1	3.766990	1.635485	7.280791
6	1.946284	1.860407	4.368877
6	2.758365	1.934928	3.336975
79	-0.024837	1.887291	3.589184
15	-2.313938	1.947974	2.979414
6	1.493586	0.863897	-1.788667
6	1.176153	-0.236380	-0.984791
6	1.511477	0.715358	-3.180770
6	0.853334	-1.461439	-1.562238
1	1.184896	-0.128889	0.102073
6	1.186432	-0.508421	-3.754632
1	1.796795	1.549980	-3.821197
6	0.851646	-1.594708	-2.947763
1	0.605683	-2.311591	-0.929030
1	1.200794	-0.617310	-4.837560
1	0.599942	-2.551047	-3.403064
6	0.437270	3.574213	-1.310059
6	0.018498	3.855918	-2.616228
6	-0.212372	4.183963	-0.232268
6	-1.035623	4.733821	-2.837159
1	0.523550	3.399314	-3.467028
6	-1.269962	5.062179	-0.457228
1	0.117895	3.968932	0.788104
6	-1.680391	5.336561	-1.758304
1	-1.352865	4.951675	-3.855472
1	-1.771064	5.537456	0.385261
1	-2.504806	6.025691	-1.934154
6	3.274594	3.162006	-1.839218
6	4.400067	2.350433	-2.030223
6	3.327981	4.511299	-2.196665
6	5.556231	2.881173	-2.590249
1	4.370330	1.298394	-1.739599
6	4.490522	5.038741	-2.754067
1	2.461460	5.154607	-2.045962
6	5.602026	4.226334	-2.953775
1	6.424631	2.242989	-2.744170
1	4.522887	6.089699	-3.036101
1	6.508615	4.641052	-3.391183
6	-2.678603	1.911733	1.195387
6	-1.881260	1.107499	0.374256
6	-3.732513	2.641194	0.637544
6	-2.135237	1.034110	-0.991451
1	-1.052095	0.542532	0.807385
6	-3.979967	2.568896	-0.730266
1	-4.359369	3.271764	1.268700
6	-3.184104	1.766416	-1.543414
1	-1.504871	0.411918	-1.627641
1	-4.797383	3.143721	-1.162540
1	-3.373845	1.720703	-2.614603
6	-3.248093	0.561778	3.706509
6	-4.265685	-0.101300	3.016614
6	-2.941152	0.187030	5.019930
6	-4.967859	-1.131177	3.637844
1	-4.514134	0.185103	1.994651
6	-3.650041	-0.836091	5.638327
1	-2.142678	0.703536	5.556747
6	-4.662598	-1.497177	4.945523
1	-5.759373	-1.647241	3.097066
1	-3.407584	-1.121921	6.660394
1	-5.212770	-2.303417	5.427802
6	-3.108816	3.458621	3.619622
6	-2.357338	4.638709	3.649278
6	-4.438917	3.473432	4.049569
6	-2.933114	5.823070	4.097329
1	-1.313484	4.624349	3.327769
6	-5.008771	4.659097	4.504036
1	-5.032656	2.559187	4.030226
6	-4.258328	5.831733	4.526684
1	-2.343482	6.737917	4.120077

1	-6.043671	4.665983	4.841315
1	-4.705981	6.756462	4.886995

VIb



E = -2693.406748 h.
G = -2692.745832 h.

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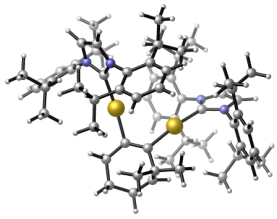
1	3.741785	4.045017	3.914791
6	3.773140	1.832387	5.541382
1	4.029999	0.850299	5.967763
1	4.055984	2.575655	6.300229
6	2.268326	1.965551	5.331649
1	1.732772	2.508544	6.113738
6	1.343335	0.942167	4.608985
6	1.864194	-0.407608	4.183331
1	1.266157	-0.811763	3.350851
1	2.908973	-0.366244	3.847423
1	1.797694	-1.129210	5.011095
6	-0.088413	0.925620	5.086007
1	-0.761110	0.618890	4.269156
1	-0.221434	0.212181	5.912026
1	-0.414267	1.915823	5.434120
79	2.284073	1.639059	1.002570
15	1.484069	0.561418	-0.954668
6	4.611194	2.089001	4.275293
1	4.743089	1.155210	3.705253
1	5.618901	2.420993	4.560257
6	2.692576	2.450337	2.872291
6	1.861487	2.143593	3.930077
79	0.640802	3.660616	2.813986
15	-1.048065	5.071913	1.972683
6	1.682614	-1.246975	-0.856492
6	0.699931	-2.137211	-1.297730
6	2.882763	-1.740173	-0.331108
6	0.918873	-3.509402	-1.212954
1	-0.236563	-1.759513	-1.709333
6	3.099651	-3.111390	-0.255916
1	3.646660	-1.044136	0.021284
6	2.116454	-3.995513	-0.694757
1	0.151448	-4.200883	-1.556449
1	4.034823	-3.491046	0.151981
1	2.283484	-5.069306	-0.629281
6	2.190153	1.069432	-2.551617
6	2.167651	0.230857	-3.670889
6	2.741556	2.350973	-2.655091
6	2.683715	0.677393	-4.882842
1	1.744830	-0.771729	-3.596720
6	3.253025	2.794875	-3.870765
1	2.770449	2.999027	-1.776899
6	3.224960	1.957285	-4.983046
1	2.666551	0.022283	-5.752016
1	3.682217	3.792417	-3.946920
1	3.630258	2.302568	-5.932624
6	-0.312891	0.867003	-1.060852
6	-0.968407	1.156863	-2.259296
6	-1.042916	0.836411	0.136162
6	-2.336638	1.423668	-2.257460
1	-0.414419	1.180955	-3.198196
6	-2.408243	1.095062	0.132977
1	-0.531072	0.620076	1.078150
6	-3.054520	1.395759	-1.066112
1	-2.841479	1.654462	-3.194057
1	-2.968601	1.075803	1.068062
1	-4.122119	1.610112	-1.067730
6	-1.228586	6.621010	2.905153
6	-0.080164	7.194874	3.461333
6	-2.464213	7.259319	3.045021
6	-0.167054	8.400637	4.148003
1	0.883097	6.692236	3.354469
6	-2.546500	8.461880	3.740371
1	-3.363636	6.820416	2.612676
6	-1.400929	9.031345	4.290825
1	0.728349	8.843694	4.580235
1	-3.510458	8.954771	3.853537
1	-1.470462	9.970893	4.836256
6	-0.724444	5.539380	0.242394
6	-0.808847	6.860421	-0.201959
6	-0.393091	4.520462	-0.660664
6	-0.556571	7.160351	-1.539059
1	-1.072819	7.659082	0.491014
6	-0.155737	4.825098	-1.995342
1	-0.335286	3.482353	-0.320157
6	-0.229981	6.146590	-2.433804
1	-0.618800	8.192224	-1.879914
1	0.091272	4.028469	-2.696677
1	-0.033772	6.384391	-3.477911
6	-2.677870	4.263443	1.979896
6	-3.004047	3.445686	3.067804
6	-3.606103	4.459350	0.954050
6	-4.249385	2.829633	3.128188
1	-2.278254	3.296797	3.870023
6	-4.851826	3.840898	1.019365
1	-3.359414	5.095198	0.103293
6	-5.172356	3.025574	2.101817
1	-4.500659	2.196643	3.977411
1	-5.575043	3.997215	0.220715
1	-6.146358	2.541589	2.148288

$TS_{IVc\text{-}VIc}$



E = -2940.278953 h.
G = -2939.037598 h.

The energy of **$TS_{IVc\text{-}VIc}$** was calculated by freezing the following distance: *d*(C8-C55). The value of this distance was taken from the optimized geometry using a simplified ligand (Me instead of *i*Pr) and B3LYP as functional.

6	0.695199	-0.419747	0.303709
6	0.222756	-0.155732	1.706398
1	0.870498	0.626407	2.136046
1	-0.744557	0.363171	1.567995
6	-0.544363	-2.525559	2.036319
1	-0.566867	-3.368621	2.747049
1	-1.595010	-2.331835	1.767025
6	0.171150	-2.979205	0.810024

1	-0.439627	-3.558247	0.114524
6	1.564350	-2.945641	0.486010
6	2.673294	-2.596147	1.457983
1	3.614518	-2.491817	0.898754
1	2.518965	-1.665479	2.007570
1	2.806439	-3.411960	2.183858
6	2.037370	-4.015184	-0.479506
1	2.821738	-3.628843	-1.144707
1	2.457429	-4.851517	0.100045
1	1.224005	-4.411934	-1.101305
6	2.087916	2.936925	-1.675972
7	1.855248	4.273198	-1.599251
7	3.316848	2.839107	-2.245006
6	3.849554	4.089970	-2.514773
1	4.828199	4.209559	-2.961695
6	2.931058	4.993550	-2.104757
1	2.934632	6.076374	-2.109438
6	0.821858	4.892636	-0.807104
6	-0.414490	5.216894	-1.392640
6	-1.355819	5.842683	-0.573298
6	0.155416	5.809443	1.303407
6	-1.077171	6.133291	0.758396
1	-2.329500	6.112482	-0.975207
1	0.369859	6.047641	2.345277
1	-1.831928	6.622606	1.372281
6	4.054974	1.614482	-2.392184
6	4.102634	1.004318	-3.651212
6	4.720074	1.097579	-1.265786
6	4.881755	-0.147426	-3.776858
6	5.477430	-0.060568	-1.444379
6	5.566952	-0.673041	-2.689726
1	4.956600	-0.632848	-4.748315
1	6.016166	-0.484206	-0.597212
1	6.175903	-1.568158	-2.811965
6	-0.700299	4.930936	-2.854724
1	-0.348706	3.906613	-3.066670
1	3.804646	2.455317	0.091727
6	4.670497	1.779624	0.085852
6	3.371254	1.564356	-4.851638
1	2.634472	2.300607	-4.493976
6	0.044581	-1.292831	2.702366
1	0.989907	-1.543975	3.196463
1	-0.630844	-0.960490	3.501767
6	1.136048	5.183983	0.529369
6	2.484279	4.875293	1.147964
1	3.116467	4.386857	0.393698
6	0.936092	-1.639383	-0.303426
79	1.161596	1.276733	-0.799941
79	0.552370	-1.848751	-2.351679
6	-0.169556	-2.234749	-4.258208
6	-1.592539	-2.285238	-6.018444
1	-2.429160	-1.956784	-6.621650
6	-0.737765	-3.323108	-6.160004
1	-0.665976	-4.097911	-6.913454
7	-1.232009	-1.628442	-4.848302
7	0.128116	-3.281332	-5.074362
6	0.960476	-4.397737	-4.694620
6	2.331387	-4.391442	-5.003302
6	0.335834	-5.468892	-4.036452
6	3.082390	-5.497411	-4.601432
6	1.133602	-6.554470	-3.664132
6	2.492638	-6.566811	-3.936460
1	4.148404	-5.531205	-4.815606
1	0.674173	-7.401932	-3.155606
1	3.100007	-7.420417	-3.638861
6	-2.029539	-0.586547	-4.253584
6	-1.957978	0.710966	-4.779714
6	-2.905624	-0.931936	-3.205810
6	-2.817087	1.672492	-4.242444
6	-3.732585	0.072523	-2.700784
6	-3.695273	1.361908	-3.215713
1	-2.798090	2.683926	-4.644009
1	-4.431524	-0.163342	-1.899583
1	-4.362730	2.125478	-2.817962
6	-1.017548	1.103391	-5.899763
1	-0.295779	0.286337	-6.051240
6	-3.033732	-2.338837	-2.657839
1	-2.124992	-2.901491	-2.914546
6	-1.148788	-5.511858	-3.737586
1	-1.607084	-4.569781	-4.069131
6	2.960713	-3.260404	-5.788356
1	2.529693	-2.316347	-5.419769
6	0.057975	5.895819	-3.770146
1	-0.235234	6.934495	-3.556545
1	1.146362	5.823764	-3.662667
1	-0.183515	5.688359	-4.822290
6	-2.180115	4.999493	-3.206719
1	-2.317653	4.715590	-4.258936
1	-2.793754	4.331520	-2.587753
1	-2.572720	6.021337	-3.103003
6	3.202364	6.155512	1.568490
1	3.311596	6.852888	0.726415
1	2.658605	6.677921	2.368541
1	4.207165	5.921275	1.947421
6	2.358163	3.911429	2.324286
1	3.354590	3.657415	2.714253
1	1.782461	4.355442	3.149293
1	1.858659	2.977681	2.027097
6	5.918660	2.630964	0.309649
1	6.045327	3.379484	-0.485574
1	5.852459	3.164954	1.269302
1	6.824850	2.007249	0.332420
6	4.455082	0.798762	1.232253
1	5.301039	0.109049	1.362331
1	4.333542	1.344964	2.178505
1	3.548042	0.199057	1.065067
6	4.336079	2.287790	-5.790423
1	4.882131	3.091768	-5.278354
1	5.078381	1.588804	-6.203644
1	3.789829	2.734248	-6.633353
6	2.610370	0.479963	-5.607067
1	2.031839	0.921802	-6.429711
1	3.296661	-0.253845	-6.055422
1	1.916200	-0.060693	-4.943649
6	-3.147718	-2.362576	-1.135932
1	-4.101788	-1.945203	-0.784810
1	-3.096352	-3.397929	-0.769111
1	-2.333618	-1.789977	-0.664253
6	-4.218323	-3.051130	-3.310207
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1	-4.310607	-4.080646	-2.934673
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1	0.337154	2.236825	-4.609443
1	0.487976	2.605603	-6.346602
1	-0.890189	3.231386	-5.430575
6	-1.781625	1.311016	-7.206881
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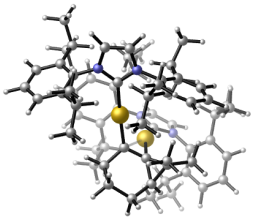
1	-2.496942	2.141641	-7.116244
1	-1.089075	1.554281	-8.024299
6	-1.826375	-6.641636	-4.509822
1	-1.649521	-6.554754	-5.590722
1	-1.454289	-7.624660	-4.187150
1	-2.912157	-6.623498	-4.340056

6	-1.418055	-5.636292	-2.241105
1	-2.499881	-5.646366	-2.045521
1	-1.000617	-6.564830	-1.825646
1	-0.978668	-4.791034	-1.691485
6	4.471965	-3.175225	-5.622924
1	4.848069	-2.275522	-6.129235
1	4.772548	-3.128095	-4.567185
1	4.980920	-4.032234	-6.086875
6	2.628152	-3.386319	-7.276608
1	3.025443	-4.330645	-7.677869
1	1.548647	-3.365850	-7.471750
1	3.086042	-2.562278	-7.841899

VIc



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G = -2939.084543 h.

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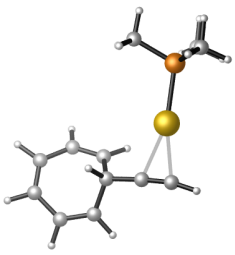
1	-1.149626	-1.454423	0.667687
6	0.951576	-2.589496	1.969679
1	1.799080	-2.752739	2.653949
1	0.165345	-3.290201	2.287158
6	1.315813	-2.951796	0.534444
1	0.980556	-3.937906	0.198987
6	2.575608	-2.472314	-0.235124
6	3.663756	-1.726661	0.491353
1	4.242579	-1.103020	-0.208645
1	3.265602	-1.068630	1.274893
1	4.366964	-2.432076	0.960275
6	3.082697	-3.417133	-1.295255
1	3.621099	-2.858342	-2.077913
1	3.781564	-4.155026	-0.873426
1	2.260783	-3.960869	-1.781019
6	2.556594	2.904952	-1.362598
7	2.234149	4.211281	-1.200694
7	3.766815	2.924337	-1.975367
6	4.189132	4.224542	-2.208073
1	5.139256	4.436061	-2.683018
6	3.224881	5.036758	-1.715471
1	3.142331	6.115459	-1.674968
6	1.097375	4.691230	-0.462845
6	0.012460	5.228458	-1.168596
6	-1.047611	5.747517	-0.421404
6	0.053777	5.156563	1.637732
6	-1.028698	5.711582	0.965917
1	-1.900720	6.187686	-0.935887
1	0.059068	5.140291	2.726821
1	-1.864547	6.121967	1.530549
6	4.623065	1.774728	-2.100728
6	4.502764	0.934828	-3.216073
6	5.558666	1.554966	-1.076361
6	5.383846	-0.146464	-3.300886
6	6.413038	0.458747	-1.209036
6	6.332385	-0.380382	-2.312982
1	5.338496	-0.808322	-4.165769
1	7.150383	0.260016	-0.431176
1	7.012734	-1.225865	-2.403010
6	-0.021797	5.280745	-2.680748
1	0.748775	4.593778	-3.067871
1	4.943453	3.268426	0.045130
6	5.647499	2.431622	0.157570
6	3.500505	1.190428	-4.320171
1	2.770499	1.932063	-3.962574
6	0.412758	-1.156874	2.134009
1	1.241949	-0.447663	2.293354
1	-0.219795	-1.099227	3.030733
6	1.145837	4.637146	0.941164
6	2.352904	4.119730	1.698116
1	2.936978	3.470910	1.029301
6	1.262744	-1.824521	-0.417504
79	1.528321	1.177729	-0.814737
79	0.061207	-1.756239	-2.248957
6	-0.889355	-2.323302	-3.997676
6	-2.295782	-2.497694	-5.753568
1	-3.101349	-2.183642	-6.405636
6	-1.517047	-3.605275	-5.747943
1	-1.499860	-4.477363	-6.389591
7	-1.896100	-1.724488	-4.673643
7	-0.654845	-3.478473	-4.669638
6	0.206587	-4.530931	-4.194129
6	1.516374	-4.633178	-4.692106
6	-0.319486	-5.418122	-3.241370
6	2.306364	-5.673229	-4.196974
6	0.519404	-6.431445	-2.771454
6	1.816873	-6.560120	-3.245398
1	3.325059	-5.795247	-4.560441
1	0.140941	-7.134518	-2.029413
1	2.455257	-7.360153	-2.873449
6	-2.584393	-0.526527	-4.273996
6	-2.150073	0.704335	-4.783688
6	-3.696367	-0.655232	-3.427747
6	-2.905438	1.831784	-4.457649
6	-4.399539	0.508628	-3.109572
6	-4.014766	1.738635	-3.626640
1	-2.615357	2.801029	-4.859954
1	-5.266773	0.445178	-2.452450
1	-4.583245	2.634684	-3.380476
6	-0.936715	0.827604	-5.679470
1	-0.350414	-0.101685	-5.594512
6	-4.151180	-1.982755	-2.860203
1	-3.480638	-2.771375	-3.230578
6	-1.743261	-5.336996	-2.730788
1	-2.245867	-4.493307	-3.223742
6	2.051352	-3.697322	-5.756843
1	1.540109	-2.726161	-5.647587
6	3.248985	5.290666	2.101860
1	3.563256	5.877800	1.226985
1	2.719847	5.968015	2.788547
1	4.154487	4.933054	2.612630
6	1.978548	3.273654	2.909507
1	2.884349	2.840219	3.356108
1	1.483070	3.863817	3.693027
1	1.307856	2.446937	2.631915
6	-1.363489	4.815053	-3.233326
1	-2.181591	5.492930	-2.952487
1	-1.329797	4.790098	-4.331550
1	-1.615736	3.808139	-2.872259
6	0.301946	6.688759	-3.179552
1	-0.451004	7.408452	-2.825445
1	1.283712	7.034405	-2.827582
1	0.305283	6.719304	-4.277800
6	7.039663	3.034586	0.324380
1	7.798614	2.261287	0.509615
1	7.344902	3.597366	-0.568795

1	7.054277	3.723793	1.180140
6	5.228449	1.659196	1.407195
1	5.886722	0.795964	1.585964
1	5.281609	2.306534	2.294446
1	4.196957	1.285359	1.319924
6	4.205357	1.785949	-5.537798
1	4.730395	2.716459	-5.278647
1	4.947133	1.083989	-5.946663
1	3.483070	2.012172	-6.334721
6	2.729023	-0.071264	-4.696031
1	1.983233	0.155228	-5.470700
1	3.391405	-0.844804	-5.106215
1	2.197924	-0.500560	-3.827430
6	-2.521796	-6.599071	-3.095741
1	-3.571166	-6.504068	-2.784537
1	-2.503943	-6.782013	-4.179308
1	-2.105791	-7.486617	-2.598092
6	-1.791023	-5.079292	-1.226555
1	-1.281086	-5.875916	-0.665435
1	-1.314368	-4.120434	-0.967926
1	-2.832867	-5.045210	-0.878441
6	3.550675	-3.447993	-5.632823
1	3.856970	-2.657186	-6.330990
1	3.834532	-3.140231	-4.616664
1	4.136103	-4.341588	-5.890667
6	1.740539	-4.244880	-7.151384
1	2.217613	-5.226263	-7.291608
1	0.663171	-4.371054	-7.320296
1	2.126675	-3.567601	-7.925439
6	-5.562873	-2.332979	-3.323559
1	-5.637442	-2.346581	-4.419810
1	-5.851650	-3.326103	-2.952499
1	-6.299674	-1.609954	-2.945679
6	-4.058651	-1.984824	-1.336436
1	-3.032459	-1.776728	-0.997911
1	-4.718414	-1.225023	-0.894210
1	-4.362775	-2.961048	-0.933823
6	-1.359212	0.979872	-7.139836
1	-1.949567	1.897011	-7.281524
1	-0.478782	1.040979	-7.794351
1	-1.972336	0.131107	-7.473647
6	-0.033129	1.980663	-5.251695
1	0.248651	1.898868	-4.189794
1	0.886817	1.986841	-5.853031
1	-0.518717	2.955356	-5.400592

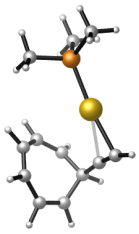
IXa



E = -944.012517 h.
G = -943.807500 h.

6	1.642572	2.726378	-1.017737
6	2.241602	2.866060	1.324457
6	0.514222	3.459220	-1.086170
1	2.355758	2.701994	-1.841353
6	1.264923	3.630768	1.852777
1	3.269740	2.928163	1.683657
6	-0.404572	3.671715	0.002887
1	0.281091	3.959213	-2.027746
6	-0.069383	3.747345	1.322544
1	1.502386	4.241360	2.725725
1	-1.428014	3.936207	-0.267320
1	-0.845815	4.070138	2.017589
6	2.981968	0.921619	-0.017654
6	3.867438	0.116201	-0.291722
1	4.611638	-0.514321	-0.748598
6	1.922092	1.899896	0.212088
1	0.999876	1.350466	0.478787
15	3.916081	-0.902620	4.164086
79	3.702206	-0.204704	1.956090
6	2.407734	-0.630099	5.139659
1	1.568994	-1.169830	4.684695
1	2.556712	-0.990153	6.166447
1	2.166112	0.439282	5.161719
6	5.238081	-0.060796	5.081970
1	5.046667	1.018501	5.102266
1	5.276042	-0.441578	6.111348
1	6.204238	-0.237370	4.594611
6	4.271581	-2.677166	4.322291
1	5.213618	-2.918433	3.816321
1	4.351596	-2.946326	5.384070
1	3.465216	-3.259020	3.860753

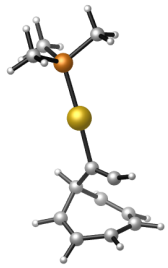
Xa



E = -944.014585 h.
G = -943.808236 h.

6	-0.884899	1.614596	-2.595764
1	-1.783826	1.631735	-3.189518
6	0.172786	1.873053	-2.023569
6	1.440781	2.344590	-1.437464
6	1.233697	3.605748	-0.631912
6	2.158837	1.338597	-0.570853
1	2.083893	2.580152	-2.296602
6	0.495851	3.656092	0.495167
1	1.691437	4.513977	-1.021562
6	1.655426	0.845892	0.580792
1	3.135597	1.005219	-0.919577
6	-0.062685	2.539042	1.211704
1	0.320842	4.639888	0.934724
6	0.456710	1.281439	1.252808
1	2.219656	0.050930	1.074605
1	-0.892555	2.761436	1.883533
1	0.012637	0.578054	1.959769
79	-0.616385	-0.353249	-1.528686
15	-0.758638	-2.492207	-0.623022
6	-1.053882	-2.478910	1.171801
1	-1.970046	-1.922219	1.401793
1	-1.151069	-3.508658	1.541697
1	-0.210063	-1.995095	1.679027
6	-2.079651	-3.528555	-1.318514
1	-1.921118	-3.666335	-2.394357
1	-2.079343	-4.508532	-0.823021
1	-3.052190	-3.046293	-1.164356
6	0.773091	-3.448671	-0.829939
1	0.664403	-4.435696	-0.360498
1	0.995616	-3.577162	-1.895638
1	1.606563	-2.912712	-0.358679

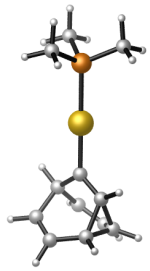
$TS_{Xa\text{-}XIa}$



E = -943.992296 h.
G = -943.787211 h.

6	-0.829980	1.701179	0.310644
1	-1.886847	1.847148	0.467119
6	0.218975	1.045620	0.010694
6	1.653171	1.561913	-0.001801
6	1.792369	2.748489	-0.914355
6	2.033764	2.124233	1.340272
1	2.347054	0.771021	-0.295681
6	0.913486	3.772443	-0.884810
1	2.608391	2.734447	-1.635388
6	1.219656	2.967501	2.008703
1	2.973956	1.790288	1.776322
6	-0.108429	3.910886	0.112034
1	0.960983	4.540370	-1.656764
6	0.029862	3.535920	1.441596
1	1.455692	3.237478	3.037853
1	-0.984552	4.508708	-0.142532
1	-0.746649	3.871287	2.130105
79	-0.288106	-0.946244	-0.513357
15	-0.705734	-3.167615	-1.129643
6	-0.963389	-4.300617	0.272279
1	-1.841807	-3.988382	0.849343
1	-1.120140	-5.322343	-0.099471
1	-0.087386	-4.287046	0.931470
6	-2.176743	-3.399214	-2.175726
1	-2.064747	-2.833239	-3.107950
1	-2.303151	-4.464369	-2.412275
1	-3.069441	-3.038512	-1.651358
6	0.651839	-3.921782	-2.079554
1	0.401317	-4.961196	-2.331661
1	0.819001	-3.356902	-3.004254
1	1.575058	-3.907324	-1.487964

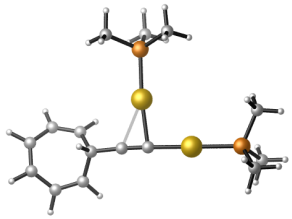
XIa



E = -944.030706 h.
G = -943.823634 h.

6	-0.647776	2.022742	0.297965
1	-1.711022	1.799190	0.284658
6	0.312381	1.053333	0.004685
6	1.726068	1.521806	0.069646
6	1.925992	2.736346	-0.835067
6	2.021204	2.156169	1.426221
1	2.440215	0.728777	-0.164586
6	0.956195	3.651819	-0.906810
1	2.887442	2.838018	-1.333299
6	1.079283	2.906143	2.004819
1	3.019677	2.023770	1.836726
6	-0.260878	3.506316	-0.105911
1	1.059894	4.553621	-1.507128
6	-0.199613	3.139759	1.331560
1	1.248097	3.407431	2.956175
1	-1.140031	4.076179	-0.402237
1	-1.040936	3.477624	1.934408
79	-0.168805	-0.880591	-0.515657
15	-0.700928	-3.109019	-1.129761
6	-0.862443	-4.240386	0.288895
1	-1.633964	-3.873009	0.975858
1	-1.137044	-5.245452	-0.058774
1	0.088988	-4.294745	0.831342
6	-2.273326	-3.295584	-2.030336
1	-2.244470	-2.718911	-2.962355
1	-2.449989	-4.353778	-2.265582
1	-3.099872	-2.921823	-1.414228
6	0.536215	-3.907262	-2.202033
1	0.229900	-4.935838	-2.435807
1	0.640966	-3.342269	-3.136020
1	1.507831	-3.928122	-1.694466

XIIa

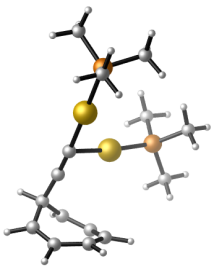


E = -1540.227874 h.
G = -1539.933930 h.

6	1.451923	3.047603	-0.959651
6	2.071285	2.902159	1.364457
6	0.313343	3.769528	-0.930873
1	2.161428	3.140226	-1.781941
6	1.091273	3.578787	1.998782
1	3.103579	2.935754	1.716513
6	-0.597353	3.830272	0.183552
1	0.063929	4.379639	-1.800781
6	-0.250135	3.741466	1.499984
1	1.328872	4.079979	2.939017
1	-1.626910	4.113003	-0.042186
1	-1.024515	3.959619	2.237149
6	2.809740	1.125693	-0.197770
6	3.692656	0.335158	-0.564543
6	1.750084	2.071254	0.148285
1	0.823816	1.504502	0.360387
15	4.135761	-0.926462	3.790638
79	3.838447	-0.198130	1.606094
6	2.615757	-0.817483	4.784677
1	1.826258	-1.423132	4.324064
1	2.803100	-1.179396	5.804714
1	2.275426	0.224380	4.826789
6	5.375261	0.011522	4.735515
1	5.097242	1.071625	4.766525
1	5.439092	-0.377561	5.760703
1	6.356211	-0.078907	4.253938
6	4.661910	-2.661722	3.937774
1	5.625886	-2.802872	3.434273

1	4.763709	-2.932034	4.997510
1	3.919922	-3.318201	3.468255
79	5.115842	-0.983563	-1.239136
15	6.744729	-2.488579	-2.008321
6	7.386600	-3.620823	-0.733254
1	8.132889	-4.298460	-1.169599
1	7.853233	-3.044666	0.074860
1	6.565058	-4.212955	-0.312828
6	6.176777	-3.586267	-3.345534
1	5.862386	-2.988158	-4.209090
1	6.989311	-4.260214	-3.648757
1	5.321448	-4.180909	-3.003596
6	8.229561	-1.682104	-2.687539
1	8.944539	-2.437393	-3.041017
1	7.948674	-1.033124	-3.525720
1	8.706219	-1.066219	-1.915712

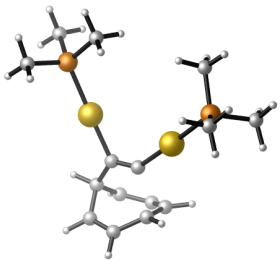
XIIIa



E = -1540.229377 h.
G = -1539.933229 h.

6	-0.564012	1.508452	1.232114
6	0.791483	1.897952	1.651000
6	1.885390	1.119953	0.957634
6	1.053420	3.368181	1.417627
1	0.862603	1.699573	2.729304
6	2.100392	1.149309	-0.374806
1	2.520473	0.500258	1.590631
6	1.049577	3.943928	0.198299
1	1.225401	3.980783	2.302040
6	1.465032	2.019566	-1.330464
1	2.857884	0.471441	-0.774365
6	0.991084	3.269236	-1.072203
1	1.132964	5.031774	0.156630
1	1.493245	1.698807	-2.373502
1	0.668616	3.868202	-1.925167
79	-1.054679	-0.499548	-0.233633
15	-0.610767	-2.382206	-1.514319
6	-0.694768	-3.953641	-0.600921
1	-1.693456	-4.080114	-0.166258
1	-0.484311	-4.792499	-1.278257
1	0.042979	-3.950229	0.210182
6	-1.759622	-2.600153	-2.908318
1	-1.703153	-1.733639	-3.577767
1	-1.502743	-3.508422	-3.470206
1	-2.786740	-2.685383	-2.532930
6	1.042449	-2.381470	-2.274406
1	1.163100	-3.266648	-2.913721
1	1.173309	-1.476330	-2.879771
1	1.809657	-2.396572	-1.491029
6	-1.744227	1.258851	0.944112
79	-3.744556	0.983437	0.547220
15	-6.033444	0.693789	0.126481
6	-6.982592	0.090612	1.559144
1	-8.040032	-0.033007	1.289195
1	-6.581493	-0.872543	1.896626
1	-6.902634	0.809498	2.383471
6	-6.416157	-0.495163	-1.199260
1	-7.503409	-0.575036	-1.332961
1	-5.961470	-0.162376	-2.140087
1	-6.010869	-1.481773	-0.944286
6	-6.896827	2.216285	-0.376038
1	-6.451385	2.609459	-1.297722
1	-7.961185	2.007892	-0.550064
1	-6.801696	2.975968	0.408986

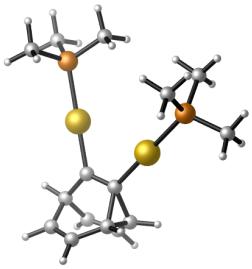
$TS_{XIIIa\text{-}XIVa}$



E = -1540.194785 h.
G = -1539.898229 h.

6	0.176894	1.004740	-0.132601
6	1.562613	1.609649	0.053924
6	1.826595	2.796166	-0.814216
6	1.651157	2.235767	1.433265
1	2.346997	0.858619	-0.076700
6	0.901814	3.774801	-0.997090
1	2.776523	2.836501	-1.346469
6	0.623452	2.970300	1.885043
1	2.547157	2.052106	2.023114
6	-0.310390	3.839664	-0.262365
1	1.068029	4.532434	-1.762586
6	-0.495780	3.322722	1.027299
1	0.602750	3.335876	2.910986
1	-1.151109	4.376473	-0.705586
1	-1.426048	3.605259	1.521989
79	-0.206758	-1.020369	-0.543840
15	-0.700747	-3.273003	-0.996123
6	-0.306838	-4.436779	0.349607
1	-0.850231	-4.150575	1.258227
1	-0.591005	-5.458665	0.063740
1	0.768152	-4.409231	0.564531
6	-2.476079	-3.542847	-1.313396
1	-2.795948	-2.933309	-2.167529
1	-2.673561	-4.601657	-1.530387
1	-3.053696	-3.241878	-0.430331
6	0.132230	-3.980831	-2.454262
1	-0.183240	-5.022628	-2.601481
1	-0.119110	-3.397363	-3.348087
1	1.219115	-3.950305	-2.312742
6	-0.960227	1.621814	0.064994
79	-2.985136	1.397032	-0.217381
15	-5.283116	1.076348	-0.601905
6	-6.300867	0.844775	0.890866
1	-7.351778	0.690350	0.611437
1	-5.944129	-0.028314	1.450238
1	-6.225532	1.727256	1.537041
6	-5.654527	-0.385873	-1.623236
1	-6.735614	-0.459411	-1.804215
1	-5.132198	-0.310238	-2.584555
1	-5.313200	-1.293092	-1.110260
6	-6.086837	2.450495	-1.487785
1	-5.598703	2.601592	-2.458092
1	-7.150073	2.226904	-1.649831
1	-5.998165	3.375177	-0.905016

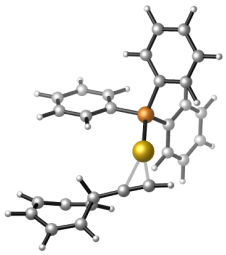
XIVa



E = -1540.208425 h.
G = -1539.908711 h.

6	0.221612	1.164345	-0.206312
6	1.633833	1.635441	-0.041303
6	1.917833	2.814065	-0.959249
6	1.798626	2.310529	1.314110
1	2.364173	0.832655	-0.179270
6	0.952101	3.720372	-1.151097
1	2.917147	2.905862	-1.379529
6	0.797357	3.070026	1.771906
1	2.751765	2.198322	1.826504
6	-0.331580	3.596687	-0.464711
1	1.103926	4.592397	-1.785271
6	-0.408877	3.273106	0.970713
1	0.866218	3.597870	2.721872
1	-1.167739	4.173877	-0.858357
1	-1.295211	3.643027	1.485204
79	-0.335113	-0.789217	-0.560249
15	-1.034150	-3.027770	-0.897802
6	-0.944418	-4.053546	0.606035
1	-1.590129	-3.629436	1.384475
1	-1.268207	-5.080064	0.386569
1	0.085767	-4.073738	0.981235
6	-2.762528	-3.200516	-1.450415
1	-2.892288	-2.695394	-2.415489
1	-3.026497	-4.261203	-1.559851
1	-3.432277	-2.738948	-0.713329
6	-0.074328	-3.963141	-2.132317
1	-0.455873	-4.990033	-2.212004
1	-0.150205	-3.474151	-3.110944
1	0.981735	-3.990972	-1.838492
6	-0.809593	2.095798	-0.070667
79	-2.798143	1.490593	-0.328430
15	-5.038235	0.818850	-0.652655
6	-5.764006	-0.164741	0.700904
1	-6.808705	-0.415441	0.471464
1	-5.193198	-1.091165	0.839547
1	-5.728212	0.407600	1.635848
6	-5.343270	-0.190414	-2.140351
1	-6.412186	-0.430672	-2.223063
1	-5.028018	0.361185	-3.034421
1	-4.768632	-1.123247	-2.088292
6	-6.199381	2.212486	-0.844876
1	-5.911486	2.821572	-1.710356
1	-7.220659	1.835610	-0.993116
1	-6.176111	2.845989	0.050064

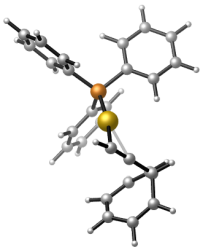
IXb



E = -1518.771350 h.
G = -1518.421072 h.

6	1.501782	2.727546	-0.781231
6	2.081836	2.837904	1.567548
6	0.237881	3.194312	-0.801565
1	2.193611	2.918517	-1.600948
6	0.965658	3.325963	2.145351
1	3.075133	3.101793	1.933537
6	-0.692026	3.117136	0.296699
1	-0.113199	3.693449	-1.706198
6	-0.366958	3.172529	1.620208
1	1.069105	3.911878	3.060181
1	-1.751922	3.160349	0.041223
1	-1.186913	3.259301	2.334757
6	3.209492	1.185309	0.110659
6	4.253573	0.607498	-0.181776
1	5.135743	0.200076	-0.646520
6	1.967268	1.902073	0.390414
1	1.184308	1.153114	0.616606
15	4.047450	-0.893379	4.152013
79	3.981137	-0.026823	1.987795
6	2.478282	-0.585503	5.011830
6	1.326173	-0.323124	4.264154
6	2.413425	-0.611466	6.409382
6	0.116039	-0.090333	4.909721
1	1.383654	-0.299293	3.173488
6	1.200912	-0.381727	7.048876
1	3.310420	-0.811892	6.996361
6	0.055035	-0.119333	6.300235
1	-0.778389	0.119951	4.326077
1	1.150723	-0.402653	8.135814
1	-0.891007	0.066947	6.805719
6	4.362087	-2.682508	4.169555
6	3.575605	-3.570914	4.905178
6	5.447095	-3.160012	3.423753
6	3.876790	-4.930918	4.894616
1	2.728883	-3.207736	5.487174
6	5.746640	-4.516203	3.424512
1	6.061528	-2.466078	2.846246
6	4.959387	-5.402211	4.159032
1	3.261421	-5.622345	5.467195
1	6.592680	-4.883772	2.846804
1	5.191705	-6.465630	4.154305
6	5.347263	-0.126239	5.165166
6	5.568453	1.248061	5.020411
6	6.084657	-0.858337	6.099570
6	6.517362	1.886009	5.810257
1	4.994118	1.815380	4.284449
6	7.037951	-0.214344	6.883241
1	5.916747	-1.928958	6.217620
6	7.253414	1.153457	6.739569
1	6.688710	2.954721	5.695401
1	7.613950	-0.785120	7.609263
1	8.002437	1.652036	7.352176

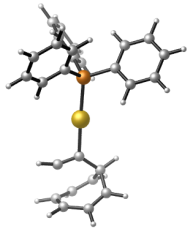
Xb



E = -1518.773660 h.
G = -1518.420864 h.

6	-0.520512	1.464781	-2.496305
1	-1.287710	1.595273	-3.241412
6	0.391389	1.601845	-1.681689
6	1.514080	1.903175	-0.776048
6	1.432679	3.332628	-0.294538
6	1.597511	1.005087	0.434418
1	2.430171	1.777157	-1.368248
6	0.409574	3.800143	0.448555
1	2.235916	4.000777	-0.601395
6	0.623192	0.906977	1.363747
1	2.509742	0.418393	0.541665
6	-0.648586	3.024769	1.042408
1	0.386535	4.872472	0.651142
6	-0.553912	1.730864	1.455527
1	0.753698	0.158724	2.149130
1	-1.555049	3.569859	1.308803
1	-1.387783	1.329100	2.033026
79	-0.374886	-0.641183	-1.704775
15	-0.544696	-2.890082	-1.098167
6	0.950347	-3.829959	-1.522877
6	2.182932	-3.168448	-1.494482
6	0.897128	-5.193425	-1.825907
6	3.353956	-3.866378	-1.766347
1	2.220353	-2.102662	-1.258403
6	2.072000	-5.885467	-2.102897
1	-0.058972	-5.716639	-1.848788
6	3.297079	-5.223794	-2.073919
1	4.311225	-3.348860	-1.745656
1	2.029138	-6.945826	-2.344523
1	4.212874	-5.769052	-2.295604
6	-0.767817	-3.031165	0.700778
6	0.066975	-3.820072	1.493753
6	-1.806323	-2.298804	1.290796
6	-0.134332	-3.871282	2.871541
1	0.874741	-4.394986	1.041587
6	-2.007894	-2.362794	2.663316
1	-2.456279	-1.676153	0.671949
6	-1.168076	-3.145918	3.454794
1	0.519306	-4.485153	3.488601
1	-2.817012	-1.795447	3.119864
1	-1.321710	-3.188414	4.531594
6	-1.951067	-3.736427	-1.873056
6	-2.282694	-3.401977	-3.190128
6	-2.662224	-4.737356	-1.204418
6	-3.317996	-4.067906	-3.836246
1	-1.727221	-2.617517	-3.707430
6	-3.699659	-5.397473	-1.855708
1	-2.405690	-5.003355	-0.178680
6	-4.026252	-5.063931	-3.167679
1	-3.576144	-3.805368	-4.860508
1	-4.253283	-6.177005	-1.335539
1	-4.840698	-5.581325	-3.671778

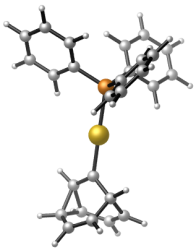
$TS_{Xb\text{-}XIb}$



E = -1518.750600 h.
G = -1518.400536 h.

6	-0.802243	1.662555	0.010343
1	-1.870883	1.804179	0.028655
6	0.281692	1.010632	-0.131810
6	1.702278	1.540626	0.010417
6	1.942751	2.693343	-0.925062
6	1.911713	2.162190	1.364002
1	2.433918	0.747826	-0.162632
6	1.057286	3.705343	-1.043941
1	2.841410	2.663754	-1.539236
6	1.015954	3.020810	1.894767
1	2.795248	1.860849	1.924678
6	-0.079887	3.869951	-0.184790
1	1.191308	4.444733	-1.833297
6	-0.100206	3.552949	1.166772
1	1.123896	3.333520	2.933136
1	-0.922998	4.446204	-0.567687
1	-0.957860	3.903438	1.742262
79	-0.218178	-0.988362	-0.617494
15	-0.691450	-3.230602	-1.137591
6	-2.185359	-3.411748	-2.158928
6	-3.236812	-2.508696	-1.968909
6	-2.316217	-4.446406	-3.089741
6	-4.411387	-2.642912	-2.700965
1	-3.130616	-1.700334	-1.242874
6	-3.492225	-4.573897	-3.822293
1	-1.502759	-5.156131	-3.241426
6	-4.536907	-3.673135	-3.630001
1	-5.225629	-1.936028	-2.552259
1	-3.591785	-5.378025	-4.549163
1	-5.454033	-3.773296	-4.207877
6	-0.953844	-4.247085	0.348799
6	-1.979777	-5.191017	0.433523
6	-0.062432	-4.088076	1.416590
6	-2.112909	-5.966743	1.582467
1	-2.677166	-5.323713	-0.393678
6	-0.193042	-4.873259	2.555557
1	0.739760	-3.350407	1.348616
6	-1.221372	-5.810336	2.639651
1	-2.915626	-6.699028	1.649015
1	0.505648	-4.749780	3.380993
1	-1.328169	-6.419267	3.535643
6	0.657192	-4.032607	-2.059321
6	1.288686	-3.303132	-3.073187
6	1.043843	-5.351378	-1.806661
6	2.294101	-3.891875	-3.831179
1	0.987749	-2.271945	-3.268432
6	2.056272	-5.933319	-2.564255
1	0.554478	-5.926474	-1.020538
6	2.679718	-5.206296	-3.574401
1	2.782907	-3.323067	-4.620062
1	2.356233	-6.960303	-2.363625
1	3.472111	-5.665255	-4.163069

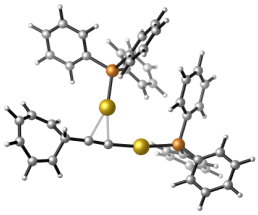
XIb



E = -1518.789483 h.
G = -1518.435158 h.

6	-0.665078	1.994757	0.056006
1	-1.726485	1.777860	-0.027752
6	0.306192	1.013574	-0.143475
6	1.715528	1.473344	0.009891
6	1.989873	2.671551	-0.896145
6	1.916633	2.127755	1.374631
1	2.438802	0.671771	-0.157903
6	1.035353	3.593214	-1.052343
1	2.985152	2.758346	-1.325986
6	0.941242	2.893412	1.871258
1	2.881960	1.994259	1.857619
6	-0.237366	3.470130	-0.339571
1	1.191022	4.482932	-1.659385
6	-0.283213	3.125163	1.103023
1	1.045136	3.408544	2.824354
1	-1.088040	4.041264	-0.707740
1	-1.163639	3.477164	1.638170
79	-0.161293	-0.932639	-0.612866
15	-0.676683	-3.196384	-1.136425
6	-2.177793	-3.370068	-2.148744
6	-3.218938	-2.455466	-1.956989
6	-2.323765	-4.405538	-3.076490
6	-4.397997	-2.579022	-2.683963
1	-3.101651	-1.646864	-1.232988
6	-3.503812	-4.522282	-3.804178
1	-1.518391	-5.124108	-3.229877
6	-4.538113	-3.609875	-3.610189
1	-5.204218	-1.863280	-2.533711
1	-3.614681	-5.327008	-4.528761
1	-5.458452	-3.701479	-4.184402
6	-0.939138	-4.206375	0.355044
6	-1.968973	-5.145073	0.449436
6	-0.042715	-4.045652	1.418543
6	-2.100707	-5.914164	1.602925
1	-2.670390	-5.278751	-0.374264
6	-0.172405	-4.823750	2.562653
1	0.763228	-3.312813	1.342792
6	-1.204179	-5.756010	2.655780
1	-2.905838	-6.643136	1.676497
1	0.530246	-4.698853	3.384543
1	-1.309797	-6.359891	3.555343
6	0.657485	-4.016862	-2.064533
6	1.286677	-3.294969	-3.085362
6	1.040345	-5.335904	-1.808172
6	2.285778	-3.891052	-3.846074
1	0.988855	-2.263460	-3.284340
6	2.046524	-5.925491	-2.568362
1	0.552723	-5.905230	-1.016717
6	2.667729	-5.205679	-3.585079
1	2.772736	-3.327773	-4.640098
1	2.343448	-6.952773	-2.364610
1	3.455464	-5.670398	-4.175511

XIIb

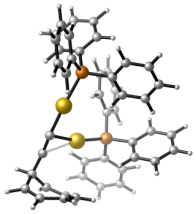


E = -2689.755157 h.
G = -2689.162782 h.

6	0.278436	2.312466	-0.896627
6	1.069971	2.165482	1.374022
6	-0.998115	2.720660	-0.746621
1	0.880622	2.634660	-1.746279
6	0.000138	2.519262	2.116246
1	2.083906	2.438257	1.671697
6	-1.815913	2.470231	0.412393
1	-1.452288	3.306724	-1.547506
6	-1.370071	2.374384	1.698675
1	0.172993	2.987656	3.087328
1	-2.896071	2.502817	0.261646
1	-2.123370	2.337639	2.487227
6	2.127585	0.748819	-0.353337
6	3.159380	0.239362	-0.818215
6	0.885909	1.369075	0.107397
1	0.150114	0.568919	0.313352
15	4.201719	-1.081044	3.435918
79	3.520520	-0.320786	1.345409
79	4.864479	-0.729520	-1.427691
15	6.802999	-1.985087	-1.873911
6	3.952028	-2.872659	3.616585
6	2.950316	-3.488824	2.859096
6	4.721996	-3.632767	4.502633
6	2.715507	-4.853705	2.992954
1	2.357846	-2.893552	2.161031
6	4.486352	-4.997916	4.630085
1	5.508941	-3.160994	5.091776
6	3.484474	-5.607462	3.877127
1	1.934753	-5.330471	2.403141
1	5.089416	-5.588500	5.317496
1	3.304126	-6.676322	3.978247
6	3.305779	-0.276723	4.800010
6	2.726944	-1.005234	5.840735
6	3.210011	1.120633	4.789618
6	2.055424	-0.338814	6.863276
1	2.797256	-2.092378	5.858048
6	2.544989	1.779887	5.815781
1	3.664730	1.691570	3.977448
6	1.964233	1.049245	6.851692
1	1.601836	-0.909741	7.671418
1	2.474901	2.866148	5.805356
1	1.437986	1.566017	7.652329
6	5.969952	-0.764284	3.729581
6	6.852802	-0.889142	2.651002
6	6.460597	-0.430816	4.995118
6	8.215009	-0.683012	2.838326
1	6.468780	-1.158071	1.662719
6	7.824824	-0.224102	5.176633
1	5.779249	-0.334128	5.840656
6	8.699989	-0.347604	4.100795
1	8.897765	-0.776280	1.994386
1	8.203985	0.037703	6.162788
1	9.765648	-0.178777	4.245944
6	6.664363	-3.066762	-3.327394
6	5.886173	-2.630696	-4.404745

6	7.327931	-4.295620	-3.400181
6	5.778578	-3.414615	-5.548399
1	5.361569	-1.675730	-4.342832
6	7.214406	-5.077127	-4.545489
1	7.934375	-4.642879	-2.562879
6	6.440465	-4.637989	-5.617360
1	5.169779	-3.073941	-6.383947
1	7.730380	-6.034036	-4.599792
1	6.351460	-5.254219	-6.510319
6	8.312612	-0.993276	-2.083715
6	9.364742	-1.403391	-2.906641
6	8.428772	0.188423	-1.342642
6	10.524690	-0.637377	-2.980367
1	9.283529	-2.320350	-3.490591
6	9.592807	0.945643	-1.413873
1	7.599124	0.517302	-0.713073
6	10.640555	0.532162	-2.233806
1	11.342096	-0.957110	-3.624178
1	9.677483	1.864604	-0.836685
1	11.549970	1.127433	-2.294265
6	7.119868	-3.076968	-0.446641
6	6.020898	-3.722547	0.135303
6	8.396336	-3.267751	0.087815
6	6.198581	-4.542521	1.243287
1	5.020915	-3.578355	-0.281102
6	8.568584	-4.087312	1.201950
1	9.260208	-2.775330	-0.359430
6	7.471993	-4.715423	1.784599
1	5.338653	-5.039214	1.692741
1	9.564290	-4.225799	1.619992
1	7.606484	-5.343980	2.663654

XIIIb



E = -2689.75457987 h.
G = -2689.163141 h.

6	-0.542321	1.367371	1.684995
6	0.784672	1.480744	2.317234
6	1.763558	0.435604	1.834847
6	1.404393	2.841340	2.101154
1	0.634789	1.336128	3.396055
6	2.191030	0.336242	0.557354
1	2.117530	-0.282943	2.574761
6	1.736709	3.330281	0.889067
1	1.555334	3.456165	2.987863
6	1.953781	1.275821	-0.507413
1	2.805238	-0.531205	0.302313
6	1.746038	2.613123	-0.359127
1	2.067153	4.369797	0.842472
1	2.093079	0.900653	-1.522884
1	1.724876	3.219439	-1.265768
79	-1.108032	-0.592163	0.308417
15	-1.007120	-2.657652	-0.754923
6	-1.697039	1.379832	1.227795
79	-3.567875	1.300000	0.378958
15	-5.656540	1.097259	-0.681672
6	-2.452585	-3.672925	-0.316910
6	-3.664830	-3.023427	-0.057535
6	-2.386180	-5.068097	-0.259166
6	-4.803039	-3.762290	0.245071
1	-3.707355	-1.930768	-0.079685
6	-3.526192	-5.803280	0.051907
1	-1.444142	-5.581551	-0.455101
6	-4.731673	-5.152277	0.301978
1	-5.745092	-3.251974	0.446926
1	-3.470909	-6.889241	0.100818
1	-5.619822	-5.731601	0.548643
6	-0.979893	-2.537686	-2.569875
6	-1.585463	-3.500922	-3.381737
6	-0.293692	-1.466499	-3.153657
6	-1.498306	-3.394440	-4.767086
1	-2.123068	-4.337475	-2.935388
6	-0.205363	-1.367561	-4.537988
1	0.170195	-0.708967	-2.518742
6	-0.807955	-2.331349	-5.344535
1	-1.971648	-4.145731	-5.396603
1	0.328429	-0.533188	-4.989341
1	-0.741850	-2.250712	-6.428104
6	0.466190	-3.612570	-0.275374
6	0.834041	-3.607094	1.075691
6	1.220267	-4.340506	-1.198743
6	1.945519	-4.326020	1.497592
1	0.246860	-3.032772	1.795598
6	2.336784	-5.054659	-0.770729
1	0.940801	-4.352405	-2.252163
6	2.699312	-5.047282	0.572804
1	2.228854	-4.318579	2.548555
1	2.924703	-5.618407	-1.492793
1	3.574985	-5.604471	0.901156
6	-5.463727	0.634890	-2.432004
6	-4.318334	-0.074741	-2.807504
6	-6.438810	0.932878	-3.389055
6	-4.155246	-0.497936	-4.122088
1	-3.546977	-0.279705	-2.060966
6	-6.270899	0.511249	-4.704108
1	-7.329928	1.495572	-3.108756
6	-5.134256	-0.206808	-5.068920
1	-3.259228	-1.049446	-4.407501
1	-7.031410	0.744008	-5.447186
1	-5.007430	-0.534027	-6.099499
6	-6.687814	-0.193219	0.087113
6	-7.518575	-1.032012	-0.660033
6	-6.654759	-0.310424	1.481969
6	-8.313459	-1.975856	-0.014660
1	-7.548571	-0.951161	-1.746426
6	-7.453912	-1.251395	2.122141
1	-6.001399	0.340557	2.066380
6	-8.283136	-2.084651	1.373177
1	-8.958903	-2.627574	-0.600945
1	-7.425422	-1.338144	3.206736
1	-8.905549	-2.824167	1.874027
6	-6.655845	2.618981	-0.662239
6	-5.996008	3.834527	-0.876652
6	-8.039353	2.603383	-0.466584
6	-6.716568	5.022715	-0.901906
1	-4.914039	3.846854	-1.021159
6	-8.754986	3.797566	-0.486208
1	-8.560570	1.660451	-0.298759
6	-8.095890	5.004093	-0.704775
1	-6.199945	5.966509	-1.067427
1	-9.832102	3.783280	-0.329562
1	-8.658904	5.935775	-0.716434

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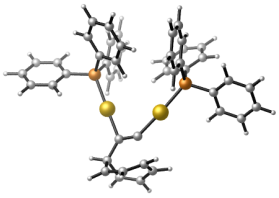
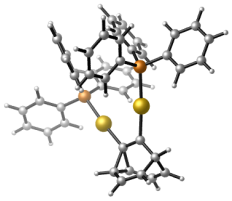


E = -2689.720607 h.
G = -2689.128040 h.

6	0.004816	1.011874	0.787008
6	1.305982	1.527028	1.384382
6	1.765714	2.820570	0.793921
6	1.068862	1.934983	2.825942
1	2.098178	0.775535	1.323041
6	0.909261	3.847546	0.556356
1	2.813694	2.905246	0.508025
6	-0.033800	2.633441	3.139197
1	1.799554	1.628762	3.572091
6	-0.441373	3.847347	0.994513
1	1.249786	4.704474	-0.024488
6	-0.920337	3.160687	2.117254
1	-0.290940	2.836978	4.178165
1	-1.155863	4.473936	0.457521
1	-1.941245	3.398513	2.419285
79	-0.331621	-0.894470	-0.028872
15	-0.819311	-3.053526	-0.851576
6	-1.149132	1.626370	0.810232
79	-3.044150	1.445927	0.044213
15	-5.144500	1.113517	-0.975923
6	-2.358544	-3.684120	-0.108111
6	-3.269649	-2.763340	0.421093
6	-2.653288	-5.051552	-0.062093
6	-4.469055	-3.202572	0.971862
1	-3.028331	-1.696006	0.417118
6	-3.856493	-5.485761	0.484765
1	-1.940664	-5.778682	-0.453929
6	-4.765676	-4.562051	0.997210
1	-5.167971	-2.478345	1.390004
1	-4.083473	-6.550035	0.513932
1	-5.706535	-4.904728	1.426061
6	-1.018441	-3.149468	-2.660180
6	-1.938246	-4.003556	-3.274893
6	-0.160764	-2.371343	-3.446710
6	-1.987891	-4.087804	-4.663623
1	-2.617103	-4.605978	-2.671592
6	-0.210314	-2.462438	-4.833789
1	0.551042	-1.696360	-2.967580
6	-1.122616	-3.323025	-5.442081
1	-2.706091	-4.754649	-5.137404
1	0.460017	-1.856779	-5.441149
1	-1.163275	-3.392652	-6.527771
6	0.466814	-4.281207	-0.444734
6	0.996178	-4.262118	0.851560
6	0.927670	-5.223236	-1.367059
6	1.972566	-5.179704	1.220337
1	0.639286	-3.523536	1.572190
6	1.912156	-6.135539	-0.994673
1	0.521912	-5.249600	-2.378283
6	2.434253	-6.114295	0.294996
1	2.380260	-5.160231	2.229484
1	2.272293	-6.865017	-1.718117
1	3.206158	-6.826421	0.581512
6	-4.941638	0.455313	-2.660850
6	-3.761475	-0.226495	-2.976643
6	-5.933751	0.610874	-3.634903
6	-3.581622	-0.759636	-4.248658
1	-2.973261	-0.324121	-2.224392
6	-5.750781	0.074380	-4.905012
1	-6.849774	1.154410	-3.399745
6	-4.577346	-0.612136	-5.210510
1	-2.656553	-1.282744	-4.490997
1	-6.525129	0.196819	-5.660363
1	-4.435061	-1.028407	-6.206733
6	-6.222884	-0.041081	-0.069206
6	-7.009571	-1.003831	-0.706183
6	-6.276898	0.089924	1.323733
6	-7.846633	-1.824637	0.046106
1	-6.972036	-1.116595	-1.789457
6	-7.120386	-0.726157	2.069412
1	-5.658651	0.838445	1.823128
6	-7.905087	-1.685068	1.429827
1	-8.455270	-2.575888	-0.454013
1	-7.161708	-0.617748	3.151727
1	-8.561372	-2.327363	2.014763
6	-6.110976	2.648887	-1.153572
6	-5.423257	3.813311	-1.514742
6	-7.493498	2.691984	-0.958231
6	-6.114188	5.007419	-1.685067
1	-4.341602	3.780747	-1.660116
6	-8.180099	3.892190	-1.124232
1	-8.038368	1.790487	-0.676705
6	-7.492712	5.047260	-1.486132
1	-5.573953	5.910392	-1.964183
1	-9.256981	3.922978	-0.968184
1	-8.032059	5.984628	-1.611343

XIVb



E = -2689.735048 h.
G = -2689.137722 h.

6	0.030950	1.142204	0.438516
6	1.372488	1.566014	0.948660
6	2.031667	2.505213	-0.054623
6	1.224706	2.509771	2.132256
1	2.018255	0.716280	1.188507
6	1.263815	3.392731	-0.696350
1	3.113378	2.458890	-0.160363
6	0.225621	3.399607	2.116535
1	1.972932	2.460572	2.920494
6	-0.168464	3.481446	-0.412942
1	1.682102	4.106046	-1.404879
6	-0.675923	3.487600	0.970522
1	0.078102	4.110738	2.927927
1	-0.793201	3.996360	-1.141939
1	-1.624725	4.003301	1.115966
79	-0.536476	-0.802996	0.063073
15	-1.158475	-3.017593	-0.574107
6	-0.895952	2.130555	0.103763
79	-2.796685	1.529203	-0.527057
15	-4.980352	0.775230	-1.069208
6	-0.756462	-3.310203	-2.327499
6	-0.421373	-2.223262	-3.141731
6	-0.761077	-4.602048	-2.866751
6	-0.102944	-2.424134	-4.482664
1	-0.399266	-1.216611	-2.718436

6	-0.456106	-4.797297	-4.209065
1	-1.002680	-5.458129	-2.235219
6	-0.126111	-3.709697	-5.016182
1	0.165164	-1.574290	-5.107985
1	-0.465583	-5.802994	-4.625223
1	0.121839	-3.868194	-6.064357
6	-2.922068	-3.409311	-0.331669
6	-3.699326	-4.072227	-1.285413
6	-3.495272	-3.042228	0.891897
6	-5.032946	-4.365913	-1.012853
1	-3.274746	-4.354866	-2.248171
6	-4.826854	-3.342024	1.159862
1	-2.894797	-2.521427	1.641760
6	-5.598322	-4.001117	0.205698
1	-5.632160	-4.881880	-1.761549
1	-5.267388	-3.044436	2.110106
1	-6.642892	-4.228211	0.413409
6	-0.243596	-4.305280	0.338551
6	1.114602	-4.077030	0.587715
6	-0.835407	-5.498168	0.760896
6	1.874766	-5.036639	1.246102
1	1.573698	-3.140899	0.262619
6	-0.071012	-6.453616	1.425852
1	-1.892588	-5.685731	0.571469
6	1.280506	-6.224398	1.667696
1	2.930532	-4.853494	1.438309
1	-0.535273	-7.381312	1.755986
1	1.873265	-6.973529	2.189825
6	-5.028563	-0.581424	-2.289371
6	-3.858719	-0.874021	-2.998543
6	-6.200184	-1.292154	-2.578878
6	-3.861741	-1.853726	-3.989393
1	-2.940645	-0.326774	-2.771116
6	-6.201988	-2.263954	-3.572563
1	-7.120926	-1.083514	-2.035331
6	-5.034026	-2.544416	-4.279485
1	-2.942954	-2.080640	-4.530618
1	-7.119290	-2.807225	-3.793929
1	-5.038361	-3.306908	-5.056919
6	-5.872798	0.242117	0.433724
6	-7.257631	0.034333	0.437773
6	-5.151695	0.072895	1.620742
6	-7.901288	-0.369440	1.601502
1	-7.843125	0.211393	-0.464936
6	-5.802326	-0.312515	2.790465
1	-4.074260	0.252486	1.629970
6	-7.174588	-0.542787	2.778514
1	-8.977296	-0.534214	1.594314
1	-5.234122	-0.433664	3.711461
1	-7.684918	-0.845666	3.691385
6	-6.030760	2.102020	-1.760446
6	-6.295994	3.206923	-0.940677
6	-6.513051	2.084002	-3.070179
6	-7.049348	4.270112	-1.422085
1	-5.916833	3.230820	0.082939
6	-7.263997	3.155832	-3.549971
1	-6.310144	1.233204	-3.719746
6	-7.534188	4.245424	-2.729243
1	-7.258627	5.121851	-0.777150
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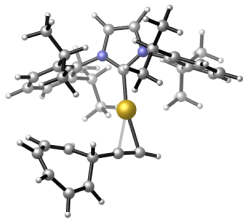
1	-8.123187	5.079495	-3.106781

IXc



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G = -1641.597475 h.

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6	2.141806	3.095458	2.114474
6	0.202482	2.857367	-0.199887
1	2.010818	1.935293	-0.839772
6	1.173745	3.967053	2.461204
1	3.190863	3.282736	2.352079
6	-0.636210	3.388649	0.844445
1	-0.127869	3.024065	-1.226511
6	-0.201003	3.884278	2.037900
1	1.446469	4.821916	3.083940
1	-1.689026	3.534658	0.598076
1	-0.935566	4.393560	2.663856
6	2.879210	0.853996	1.387464
6	3.805698	0.053938	1.264310
1	4.573846	-0.617764	0.918199
6	1.784032	1.822188	1.391771
1	0.916000	1.362135	1.903144
79	3.591278	0.185077	3.492470
6	3.749494	-0.052850	5.515401
6	3.943515	0.324138	7.723703
1	3.982610	0.928079	8.621454
6	4.007134	-1.017141	7.531752
1	4.124165	-1.841098	8.224053
7	3.787869	0.897052	6.472768
7	3.882112	-1.226206	6.169364
6	3.869485	-2.504417	5.512607
6	5.082644	-3.018902	5.035430
6	2.634497	-3.146231	5.337471
6	5.033831	-4.237932	4.355676
6	2.642507	-4.362810	4.652402
6	3.827735	-4.901405	4.165529
1	5.954360	-4.669572	3.963531
1	1.704102	-4.892595	4.489739
1	3.810736	-5.850057	3.631252
6	3.595716	2.299729	6.226825
6	4.712171	3.091095	5.922229
6	2.288719	2.802849	6.299156
6	4.484319	4.449674	5.692660
6	2.117675	4.169252	6.070064
6	3.203422	4.983824	5.771239
1	5.324300	5.098610	5.446512
1	1.116525	4.598020	6.122209
1	3.049508	6.047350	5.593850
6	1.090552	1.923847	6.592040
1	1.439312	0.890307	6.739490
6	6.105356	2.513060	5.789242
1	6.085391	1.472362	6.148511
6	1.329959	-2.546355	5.820141
1	1.560418	-1.681083	6.459515
6	6.399571	-2.290575	5.206680
1	6.233972	-1.419128	5.858897
6	0.122708	1.911098	5.410992
1	-0.709935	1.220618	5.603853
1	-0.306595	2.908643	5.237527

1	0.625252	1.594081	4.483733
6	0.384850	2.355329	7.874826
1	1.070233	2.348689	8.733615
1	-0.027990	3.369879	7.781764
1	-0.448975	1.676908	8.100557
6	7.128177	3.267068	6.633717
1	7.252317	4.303671	6.291052
1	6.839225	3.293636	7.692665
1	8.109652	2.779479	6.561262
6	6.530534	2.488431	4.320650
1	6.605294	3.507173	3.912869
1	7.514175	2.010772	4.209550
1	5.808070	1.931772	3.701178
6	7.450973	-3.167520	5.881051
1	8.366489	-2.588953	6.063463
1	7.095479	-3.551911	6.846501
1	7.726648	-4.028977	5.256597
6	6.905076	-1.768971	3.862544
1	7.094009	-2.594528	3.161074
1	6.173022	-1.089464	3.395282
1	7.846900	-1.217993	3.992490
6	0.522691	-3.528421	6.664133
1	0.197576	-4.399261	6.078242
1	1.102092	-3.896432	7.521245
1	-0.381108	-3.039670	7.051930
6	0.501841	-2.037626	4.639716
1	0.226246	-2.861886	3.965730
1	-0.428662	-1.572734	4.994227
1	1.054850	-1.291016	4.047287

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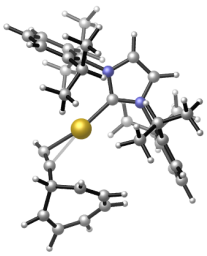

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6	-0.319551	0.207914	-1.204856
6	0.769000	1.068531	-0.703729
6	0.210653	2.392736	-0.238541
6	1.573371	0.485637	0.429570
1	1.438693	1.239662	-1.557728
6	-0.670898	2.499467	0.776593
1	0.524270	3.280166	-0.786634
6	1.036239	0.134243	1.616425
1	2.640782	0.350585	0.253271
6	-1.078643	1.447532	1.671902
1	-1.107381	3.482813	0.961596
6	-0.312503	0.386875	2.050701
1	1.684444	-0.376862	2.333107
1	-2.026798	1.593126	2.191471
1	-0.690080	-0.252124	2.852355
79	-0.274411	-2.104309	-0.877999
6	0.102657	-4.060536	-0.390280
6	0.355632	-6.024928	0.678479
1	0.447412	-6.677819	1.537478
6	0.422165	-6.274393	-0.652722
1	0.562909	-7.192239	-1.209750
7	0.148578	-4.662131	0.820730
7	0.262003	-5.056083	-1.289380
6	0.269544	-4.854656	-2.713237
6	1.449970	-4.394959	-3.316460
6	-0.915548	-5.091038	-3.424468
6	1.416088	-4.173536	-4.694521
6	-0.893723	-4.856960	-4.800810
6	0.259139	-4.402936	-5.429767
1	2.313471	-3.813144	-5.197535
1	-1.797823	-5.028244	-5.385211
1	0.256001	-4.223683	-6.503808
6	0.202369	-3.954129	2.074157
6	1.474619	-3.558575	2.518952
6	-0.977678	-3.687763	2.790293
6	1.549852	-2.852686	3.721885
6	-0.838109	-2.979110	3.987113
6	0.404160	-2.558671	4.447587
1	2.523942	-2.536194	4.094802
1	-1.733230	-2.760758	4.570168
1	0.478217	-2.008298	5.384239
6	2.750538	-3.923146	1.785733
1	2.489342	-4.433797	0.847381
6	-2.371263	-4.182230	2.437271
1	-3.045344	-3.610148	3.093674
6	-2.193852	-5.547811	-2.753495
1	-1.988642	-5.713377	-1.685801
6	2.720956	-4.121543	-2.539030
1	2.546926	-4.364691	-1.479569
6	-2.688000	-6.871882	-3.329935
1	-2.952566	-6.776394	-4.392446
1	-1.925387	-7.657977	-3.242758
1	-3.585885	-7.208499	-2.794419
6	-3.273332	-4.471036	-2.849217
1	-3.561518	-4.287122	-3.894124
1	-4.174777	-4.780998	-2.302334
1	-2.929843	-3.516249	-2.422463
6	3.867402	-5.003336	-3.027726
1	3.610557	-6.069370	-2.961528
1	4.124209	-4.783234	-4.073530
1	4.767384	-4.831398	-2.421798
6	3.098097	-2.642644	-2.613743
1	4.001094	-2.443214	-2.020089
1	3.307198	-2.336826	-3.648918
1	2.285609	-2.002640	-2.230567
6	3.577740	-2.697849	1.409719
1	3.898847	-2.131824	2.296297
1	4.484618	-3.006971	0.871444
1	3.012047	-2.015048	0.759159
6	3.572665	-4.903257	2.621403
1	3.907351	-4.440457	3.560816
1	2.990171	-5.798980	2.878073
1	4.466398	-5.223769	2.069085
6	-2.532021	-5.654710	2.816547
1	-1.912785	-6.303938	2.181044
1	-2.248487	-5.832483	3.862503
1	-3.577021	-5.969200	2.689481
6	-2.852541	-3.939999	1.009756
1	-2.666735	-2.906830	0.679312
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1	-3.935159	-4.120744	0.957447

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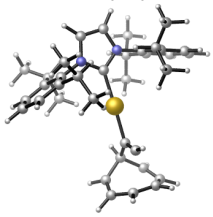

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6	-0.076755	-0.076935	-0.225113
6	1.131468	0.849366	-0.198065
6	1.118702	1.784620	-1.376175
6	1.065891	1.784687	0.977906
1	2.060605	0.273281	-0.176568
6	0.003056	2.454411	-1.733108
1	2.034317	1.871089	-1.959064
6	-0.064520	2.454712	1.285613
1	1.953636	1.869132	1.602707
6	-1.195969	2.474248	-0.943725
1	-0.012827	3.008531	-2.671353
6	-1.226965	2.476164	0.443788
1	-0.121617	3.006832	2.223487
1	-2.134499	2.687137	-1.457353
1	-2.187497	2.688125	0.915251
79	0.031249	-2.180807	-0.189664
6	0.215977	-4.228252	-0.132261
6	0.431536	-6.347702	0.604134
1	0.530981	-7.128350	1.347591
6	0.376492	-6.390242	-0.750192
1	0.418826	-7.215706	-1.449741
7	0.335871	-5.012780	0.961520
7	0.243874	-5.080159	-1.179959
6	0.140173	-4.659340	-2.548672
6	1.315502	-4.312341	-3.229613
6	-1.134142	-4.591056	-3.127750
6	1.185016	-3.890277	-4.553999
6	-1.209299	-4.163537	-4.455076
6	-0.063127	-3.819386	-5.161306
1	2.075539	-3.609116	-5.116600
1	-2.182758	-4.099500	-4.941431
1	-0.143297	-3.489705	-6.196061
6	0.328350	-4.506579	2.306152
6	1.555416	-4.190997	2.907869
6	-0.909635	-4.314875	2.934521
6	1.514789	-3.662872	4.199198
6	-0.894728	-3.782782	4.225614
6	0.303327	-3.462236	4.851651
1	2.445177	-3.397712	4.700739
1	-1.837568	-3.618908	4.747512
1	0.294086	-3.050483	5.859672
6	2.872359	-4.345830	2.175965
1	2.703956	-4.983945	1.295510
6	-2.225928	-4.643092	2.260313
1	-2.012968	-5.106543	1.284293
6	-2.396149	-4.957255	-2.374940
1	-2.124828	-5.234432	-1.344783
6	2.680232	-4.357542	-2.575161
1	2.566759	-4.757969	-1.556151
6	-3.037247	-3.374771	2.000701
1	-3.293873	-2.867115	2.941805
1	-2.479275	-2.659720	1.374109
1	-3.976980	-3.617953	1.485563
6	-3.033017	-5.649473	3.076343
1	-3.945979	-5.934422	2.536247
1	-2.455374	-6.563051	3.272470
1	-3.339122	-5.230218	4.045066
6	3.944192	-5.021621	3.025187
1	3.599018	-5.985056	3.423208
1	4.840981	-5.207822	2.419196
1	4.251919	-4.395937	3.874550
6	3.360188	-2.985305	1.675219
1	2.608949	-2.497547	1.031950
1	3.566690	-2.310894	2.519628
1	4.288775	-3.096000	1.097783
6	3.628272	-5.287725	-3.327107
1	3.210123	-6.299903	-3.415852
1	3.833788	-4.918509	-4.341808
1	4.589669	-5.362152	-2.801119
6	3.268235	-2.953064	-2.453189
1	4.242127	-2.984836	-1.945437
1	3.420601	-2.498283	-3.442746
1	2.602748	-2.289683	-1.877624
6	-3.074328	-6.168095	-3.011629
1	-3.397483	-5.949029	-4.039210
1	-2.396955	-7.032575	-3.050582
1	-3.964218	-6.459171	-2.437197
6	-3.353123	-3.770501	-2.289040
1	-3.687231	-3.448597	-3.285565
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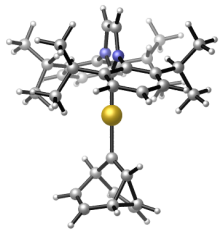

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6	-0.094478	-0.139522	0.427738
6	0.357654	0.890189	-0.552478
6	-0.757576	1.892625	-0.833980
6	1.391400	1.811363	0.090600
1	0.738756	0.445616	-1.475862
6	-1.541857	2.283237	0.174726
1	-0.825782	2.300995	-1.839752
6	1.221349	2.178666	1.363819
1	2.190582	2.189910	-0.542695
6	-1.315368	1.775061	1.530040
1	-2.326921	3.024538	0.037495
6	0.050400	1.722630	2.117360
1	1.904261	2.867258	1.857787
1	-2.126413	1.863536	2.250827
1	0.090756	1.775574	3.203941
79	0.051609	-2.137752	0.057043
6	0.210890	-4.179263	-0.276882
6	0.364728	-6.401126	0.076241
1	0.402823	-7.305862	0.670105
6	0.424379	-6.195628	-1.263993
1	0.523740	-6.881607	-2.095720
7	0.234061	-5.153430	0.659948
7	0.325040	-4.828407	-1.456887

6	0.360481	-4.158174	-2.727267
6	1.596603	-3.693526	-3.197174
6	-0.847149	-3.963842	-3.413771
6	1.601023	-3.006696	-4.413403
6	-0.787495	-3.269382	-4.623406
6	0.422156	-2.794997	-5.117407
1	2.542803	-2.626227	-4.809222
1	-1.704732	-3.088808	-5.182899
1	0.445340	-2.254320	-6.062403
6	0.153599	-4.896598	2.070989
6	1.346641	-4.681756	2.775721
6	-1.112793	-4.843079	2.670562
6	1.243624	-4.422462	4.143590
6	-1.160310	-4.577968	4.040738
6	0.004428	-4.372283	4.770437
1	2.151015	-4.258306	4.724544
1	-2.127251	-4.529311	4.541586
1	-0.054464	-4.169642	5.838793
6	2.707286	-4.718368	2.112446
1	2.567244	-4.897356	1.035592
6	-2.394799	-5.040797	1.890494
1	-2.139784	-5.195712	0.831126
6	-2.176514	-4.430578	-2.858604
1	-1.979915	-5.123117	-2.026425
6	2.888329	-3.890423	-2.431618
1	2.677631	-4.504654	-1.542967
6	3.553636	-5.864136	2.661760
1	3.757039	-5.729306	3.733794
1	3.052257	-6.833526	2.533547
1	4.520440	-5.910812	2.142230
6	3.430703	-3.382547	2.265057
1	3.651377	-3.163298	3.319538
1	4.387001	-3.400390	1.724825
1	2.829925	-2.550151	1.868795
6	3.441222	-2.551217	-1.947130
1	3.690506	-1.895413	-2.793977
1	2.714091	-2.020007	-1.311255
1	4.357847	-2.703833	-1.360543
6	3.924175	-4.639067	-3.265674
1	4.827792	-4.829961	-2.671197
1	3.536348	-5.606341	-3.613501
1	4.226509	-4.059975	-4.149561
6	-3.141471	-6.284274	2.366299
1	-2.515281	-7.183713	2.286269
1	-3.455497	-6.185927	3.415330
1	-4.044886	-6.444898	1.762545
6	-3.284518	-3.802193	1.968568
1	-4.175801	-3.931456	1.339256
1	-3.627493	-3.618147	2.996623
1	-2.752692	-2.901469	1.624413
6	-2.961853	-3.244926	-2.297210
1	-2.382292	-2.698269	-1.536295
1	-3.220195	-2.532630	-3.094803
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6	-3.008483	-5.187190	-3.889606
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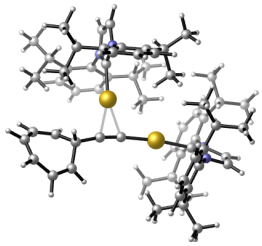

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1	2.986607	0.396465	-1.949848
6	0.531885	1.974313	0.726075
1	2.598645	2.312307	1.123802
6	-0.361000	0.524239	-1.094074
1	0.757738	0.325739	-2.933959
6	-0.508533	1.231002	0.064135
1	0.232923	2.890335	1.240650
1	-1.269733	0.144637	-1.564320
1	-1.524262	1.368911	0.438751
6	3.639927	-0.071571	0.563338
6	4.817524	-0.458344	0.687753
6	2.276889	0.305147	0.175462
1	1.580781	-0.462932	0.565340
79	4.175267	-0.006734	2.807275
6	4.102962	0.160858	4.848302
6	4.296729	0.883885	6.973706
1	4.502330	1.603968	7.755539
6	3.882241	-0.406074	7.019509
1	3.653889	-1.061471	7.850126
7	4.425378	1.212121	5.634151
7	3.774192	-0.832187	5.706294
6	3.378971	-2.149088	5.284373
6	4.371985	-3.134447	5.171426
6	2.030669	-2.373378	4.969697
6	3.973090	-4.389739	4.709958
6	1.687211	-3.646087	4.507805
6	2.647043	-4.641595	4.376723
1	4.712799	-5.182732	4.606756
1	0.651724	-3.859838	4.244404
1	2.357693	-5.627705	4.016510
6	4.817258	2.505844	5.146098
6	6.159098	2.715005	4.794174
6	3.831273	3.497696	5.042359
6	6.503462	3.983269	4.322326
6	4.229082	4.746890	4.562367
6	5.550463	4.988169	4.207932
1	7.534931	4.186857	4.036131
1	3.489501	5.541118	4.463446
1	5.842287	5.970260	3.838911
6	2.382984	3.253641	5.412330
1	2.292145	2.235914	5.819150
6	7.204848	1.621310	4.861177
1	6.767211	0.743819	5.364881
6	0.975579	-1.292060	5.081075
1	1.415724	-0.431698	5.607885
6	5.829298	-2.849226	5.475556
1	5.879900	-1.940391	6.095131
79	6.692067	-1.257320	0.643743
6	8.529077	-2.163386	0.347721
6	10.003535	-3.607943	-0.577306

1	10.309444	-4.475170	-1.148585
6	10.715989	-2.628976	0.026980
1	11.782074	-2.459140	0.105921
7	8.668844	-3.305527	-0.369791
7	9.798021	-1.754884	0.593917
6	7.574614	-3.995201	-0.996624
6	7.163500	-3.553132	-2.262899
6	6.959705	-5.054137	-0.314387
6	6.087107	-4.218485	-2.853143
6	5.893317	-5.690136	-0.951902
6	5.459906	-5.275702	-2.206041
1	5.737947	-3.901618	-3.836076
1	5.392385	-6.522889	-0.459237
1	4.624360	-5.784025	-2.685129
6	10.191911	-0.529325	1.238822
6	10.725176	-0.590854	2.536113
6	10.097706	0.667150	0.506543
6	11.218016	0.596602	3.083362
6	10.595034	1.825126	1.106826
6	11.160200	1.789667	2.375836
1	11.652615	0.585459	4.082380
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1	1.926147	5.261089	6.141138
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1	8.967769	2.873912	5.171224
1	8.168358	2.367031	6.676197
1	9.142285	1.209562	5.742077
6	7.602834	1.192725	3.449485
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1	6.607293	-4.886644	5.658635
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6	6.593921	-2.568615	4.179960
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1	-0.775513	-2.563663	5.390330
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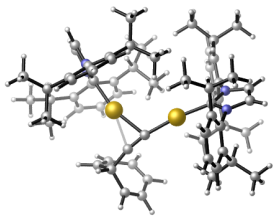
XIIIc



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6	0.016973	-4.294304	-1.816974
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6	-1.299599	-4.415193	-2.281631
6	0.719973	-3.234232	-3.839083
6	-1.576483	-3.917488	-3.557465

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6	1.622073	-3.457875	4.890243
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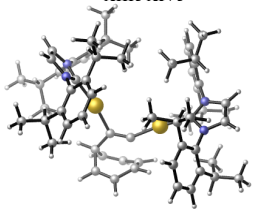

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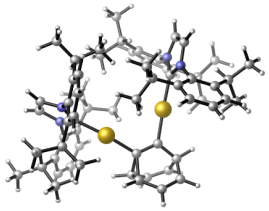
1	-6.924033	-7.372112	1.155922
1	-7.584815	-6.970400	2.742922
1	-8.568388	-6.710031	1.286925
6	-5.542387	-5.211106	2.111148
1	-5.099864	-4.205136	2.047580
1	-5.485425	-5.549702	3.156482
1	-4.919974	-5.883268	1.501837

XIVc

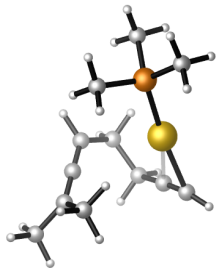


E = -2936.654772 h.
G = -2935.484436 h.

6	-0.314585	0.601177	0.064972
6	-0.607433	1.390575	-1.198104
6	-0.414067	1.696531	1.116881
1	0.689659	0.165652	0.042121
6	-1.879127	1.699672	-1.475779
1	0.234490	1.721821	-1.802766
6	-1.634462	2.092571	1.495317
1	0.505957	2.160193	1.467093
6	-2.953146	1.304577	-0.565344
1	-2.149014	2.279455	-2.357325
6	-2.826669	1.498936	0.892496
1	-1.782142	2.893293	2.218920
1	-3.971267	1.330959	-0.954617
1	-3.766386	1.629513	1.430809
6	-0.286561	-4.377772	0.877954
6	0.406996	-6.380437	1.660198
1	0.673884	-7.101158	2.422955
6	0.386546	-6.459910	0.309192
1	0.637783	-7.265516	-0.368887
7	-0.009944	-5.097819	1.990930
7	-0.037153	-5.223111	-0.153702
6	0.042126	-4.806450	-1.531583
6	1.286284	-4.345212	-1.992772
6	-1.100341	-4.850014	-2.342687
6	1.366142	-3.925603	-3.321652
6	-0.968706	-4.409112	-3.661360
6	0.249611	-3.952527	-4.147549
1	2.318924	-3.568029	-3.712099
1	-1.839614	-4.418773	-4.316347
1	0.329521	-3.616020	-5.180142
6	0.030979	-4.577423	3.332199
6	1.098026	-3.730037	3.686369
6	-0.949057	-4.985276	4.247675
6	1.155324	-3.290662	5.010119
6	-0.833624	-4.526840	5.563168
6	0.205131	-3.688791	5.942360
1	1.974534	-2.642952	5.320756
1	-1.574879	-4.834138	6.301066
1	0.277098	-3.343766	6.972700
6	2.200533	-3.339002	2.722674
1	1.884523	-3.593959	1.702004
6	-2.118877	-5.868547	3.871397
1	-2.027496	-6.147110	2.811112
6	-2.447005	-5.297974	-1.824509
1	-2.293631	-5.768179	-0.840979
6	2.518496	-4.282699	-1.113684
1	2.247778	-4.615761	-0.100646
6	-1.376352	-0.434569	0.316833
6	-2.713147	-0.023383	0.320759
79	-0.859883	-2.385096	0.662331
79	-4.329558	-1.209463	0.912260
6	-5.955031	-2.135552	1.810935
7	-6.426930	-1.697321	3.008670
7	-6.788148	-3.144720	1.460631
6	-7.536274	-2.429120	3.404317
1	-8.058149	-2.215451	4.328769
6	-7.765836	-3.339450	2.429703
1	-8.525765	-4.103011	2.320032
6	-6.794875	-3.830832	0.196156
6	-7.214072	-3.128929	-0.948768
6	-6.442911	-5.187846	0.163678
6	-7.285786	-3.842014	-2.147253
6	-6.560949	-5.859315	-1.055955
6	-6.975430	-5.195069	-2.201709
1	-7.611896	-3.329119	-3.051581
1	-6.306509	-6.918385	-1.108547
1	-7.052428	-5.733096	-3.145636
6	-6.027309	-0.453639	3.619766
6	-6.771419	0.690277	3.281221
6	-4.934285	-0.413632	4.496364
6	-6.406923	1.898479	3.877834
6	-4.606431	0.822623	5.059229
6	-5.337696	1.965277	4.762313
1	-6.965927	2.802640	3.636819
1	-3.758382	0.886491	5.740614
1	-5.068446	2.916619	5.218957
6	-7.898082	0.671876	2.266426
1	-8.067927	-0.365198	1.941937
6	-4.079795	-1.622030	4.803964
1	-4.525415	-2.493553	4.302489
6	-5.906902	-5.926030	1.371352
1	-5.838705	-5.217220	2.210083
6	-7.640298	-1.674459	-0.921475
1	-7.304022	-1.226828	0.023133
6	-3.110250	-6.333587	-2.728451
1	-3.400948	-5.901509	-3.696774
1	-2.450925	-7.190050	-2.923921
1	-4.028579	-6.711174	-2.256738
6	-3.365121	-4.090765	-1.629500
1	-4.318880	-4.404804	-1.184004
1	-2.909351	-3.337675	-0.967104
1	-3.585090	-3.602161	-2.591843
6	3.607577	-5.224161	-1.621122
1	3.247081	-6.260408	-1.681375
1	3.956048	-4.929443	-2.621290
1	4.474745	-5.204825	-0.946347
6	3.044248	-2.853891	-0.997961
1	3.894979	-2.813739	-0.303014
1	3.396305	-2.474945	-1.968108
1	2.268056	-2.164987	-0.632385
6	3.468500	-4.138285	3.019182
1	3.854377	-3.913066	4.024161
1	3.282873	-5.220647	2.966916
1	4.259879	-3.896718	2.295474
6	2.475795	-1.838270	2.730945
1	2.873038	-1.494092	3.696096
1	3.220794	-1.588094	1.962394

1	1.560717	-1.264096	2.517307
6	-2.130757	-7.159455	4.685994
1	-1.178999	-7.701123	4.598489
1	-2.307760	-6.961648	5.752794
1	-2.933460	-7.824623	4.337794
6	-3.433367	-5.106919	4.035874
1	-4.290094	-5.766698	3.837808
1	-3.545243	-4.721327	5.060059
1	-3.487977	-4.253411	3.341559
6	-4.495459	-6.443388	1.098648
1	-3.807792	-5.616123	0.863283
1	-4.103575	-6.975245	1.977022
1	-4.481972	-7.149824	0.256075
6	-6.827681	-7.066636	1.794866
1	-7.847406	-6.714054	2.001637
1	-6.892953	-7.837691	1.013875
1	-6.444011	-7.548162	2.705527
6	-9.163356	-1.564479	-0.958419
1	-9.570395	-1.977928	-1.893012
1	-9.626698	-2.107002	-0.121535
1	-9.477829	-0.512548	-0.894644
6	-6.996178	-0.860989	-2.040108
1	-7.359654	-1.158634	-3.033545
1	-7.231782	0.205247	-1.914793
1	-5.901003	-0.970370	-2.033390
6	-7.511836	1.477558	1.026669
1	-8.328139	1.466668	0.290436
1	-7.308084	2.528208	1.279361
1	-6.611101	1.064227	0.544288
6	-9.211355	1.172588	2.861045
1	-9.495860	0.595403	3.751748
1	-9.151155	2.230969	3.151605
1	-10.02053	1.077472	2.123543
6	-4.032165	-1.926089	6.298787
1	-3.551584	-1.112591	6.860809
1	-5.036736	-2.076930	6.716993
1	-3.447614	-2.839272	6.482260
6	-2.668958	-1.427931	4.245604
1	-2.064817	-2.335470	4.393041
1	-2.694407	-1.205808	3.166931
1	-2.152988	-0.597281	4.750999

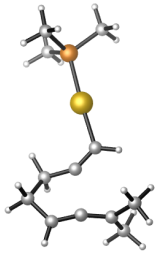
XVa



E = -946.424957 h.
G = -946.180592 h.

6	5.446909	2.029004	2.725645
79	3.478866	2.462975	1.350539
15	1.532821	2.083297	0.133433
6	1.600814	0.522555	-0.797992
1	1.794349	-0.311110	-0.111181
1	0.645325	0.353088	-1.312883
1	2.408334	0.562995	-1.538550
6	1.108769	3.355904	-1.091425
1	0.174343	3.081601	-1.599116
1	0.979836	4.325439	-0.596369
1	1.910927	3.442774	-1.833617
6	0.063773	1.933292	1.193909
1	-0.128386	2.884562	1.704647
1	-0.811632	1.668934	0.585109
1	0.227602	1.154244	1.948937
6	5.724278	0.656101	3.144523
1	6.715702	0.389405	2.751891
1	5.806882	0.652899	4.241692
6	4.710224	-0.396999	2.698252
1	5.123309	-1.382940	2.956463
1	4.626949	-0.388183	1.599101
6	3.338806	-0.256887	3.303481
1	2.593116	-0.970375	2.935788
6	2.992840	0.622169	4.213320
6	2.657081	1.505027	5.125575
6	2.140779	2.871226	4.770325
1	1.129735	3.022683	5.176962
1	2.781563	3.648031	5.214994
1	2.108551	3.034984	3.683271
6	2.776251	1.212345	6.595111
1	3.151377	0.200940	6.787610
1	3.454932	1.932543	7.075561
1	1.799351	1.320768	7.089168
6	5.323531	3.211990	2.412494
1	5.453094	4.273323	2.279191

$TS_{XVa\text{-}XVIa}$

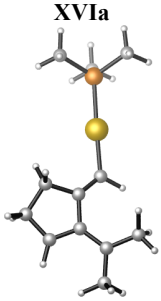


E = -946.402604 h.
G = -946.158622 h.

6	3.090737	1.034991	3.720096
79	2.175187	2.103476	1.169494
15	1.662483	2.195066	-1.117417
6	2.853442	1.326689	-2.187396
1	2.893608	0.265065	-1.916158
1	2.550779	1.417804	-3.239393
1	3.853174	1.758903	-2.060216
6	1.608666	3.889757	-1.781393
1	1.377900	3.867533	-2.855026
1	0.838122	4.469285	-1.259143
1	2.578126	4.379744	-1.631579
6	0.048208	1.481807	-1.563666
1	-0.751456	2.002123	-1.023162
1	-0.122932	1.580623	-2.644204
1	0.022134	0.420179	-1.290755
6	3.530362	-0.353172	3.469612
1	3.211533	-0.612787	2.450792
1	4.629239	-0.395680	3.496310
6	2.953906	-1.291152	4.519614
1	3.482445	-2.252279	4.524299
1	1.893545	-1.507923	4.320426
6	3.110370	-0.579228	5.829122
1	3.008604	-1.114317	6.774031
6	3.349921	0.712535	5.799664
6	3.736873	1.956873	6.117348
6	2.757099	3.062870	6.266513
1	2.799246	3.424390	7.305041
1	3.033960	3.921993	5.635610
1	1.729937	2.754238	6.047838
6	5.182431	2.312004	6.214439

1	5.831192	1.430654	6.209331
1	5.456439	2.959618	5.367226
1	5.364164	2.897055	7.126765
6	2.625508	2.128589	3.235925
1	2.436051	3.065281	3.757868

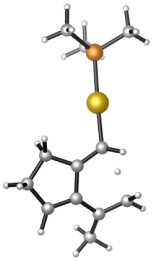
XVIa



E = -946.451495 h.
G = -946.204031 h.

6	3.026373	1.791440	3.874533
79	2.196473	1.266487	0.970158
15	1.655018	1.645940	-1.310700
6	2.586716	0.606566	-2.486099
1	2.382012	-0.452515	-2.287279
1	2.301934	0.841975	-3.520521
1	3.662389	0.780620	-2.361400
6	1.960980	3.345295	-1.900802
1	1.710716	3.436605	-2.966499
1	1.351291	4.052108	-1.324930
1	3.017505	3.602347	-1.756654
6	-0.089008	1.341119	-1.751444
1	-0.741427	1.988690	-1.153190
1	-0.259883	1.541578	-2.817834
1	-0.347275	0.297119	-1.535787
6	3.068405	3.297196	3.684604
1	4.038358	3.600590	3.261525
1	2.292103	3.648058	2.995375
6	2.926019	3.878363	5.096769
1	1.885124	4.178838	5.324324
1	3.533712	4.767121	5.312614
6	3.243732	2.757571	5.993139
1	3.405848	2.889674	7.061247
6	3.337281	1.560317	5.312304
6	3.842474	0.409721	5.949024
6	4.313251	-0.745467	5.168454
1	5.048011	-1.334229	5.729299
1	3.451061	-1.408432	4.978843
1	4.703713	-0.454353	4.185771
6	3.956581	0.279022	7.413914
1	3.467209	1.064074	7.992985
1	3.538128	-0.695224	7.708587
1	5.022183	0.227864	7.687486
6	2.680937	0.883152	2.943017
1	2.665056	-0.160629	3.273022

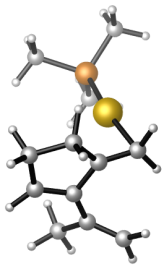
$TS_{XVIa\text{-}XVIIa}$



E = -946.402111 h.
G = -946.158971 h.

6	3.273036	2.124906	4.045267
79	2.864745	1.744236	1.046379
15	1.759568	1.667664	-1.047797
6	0.679133	0.221729	-1.310966
1	-0.105813	0.202811	-0.545226
1	0.213516	0.271422	-2.304568
1	1.264273	-0.702450	-1.232929
6	2.891945	1.635072	-2.478258
1	2.320756	1.612863	-3.416517
1	3.531154	2.526294	-2.467026
1	3.533345	0.747018	-2.426611
6	0.668827	3.088435	-1.392835
1	1.249290	4.018673	-1.365132
1	0.205725	2.981585	-2.383288
1	-0.118661	3.147322	-0.631868
6	1.964590	2.854058	4.175066
1	1.961069	3.770188	3.571791
1	1.155617	2.219977	3.780179
6	1.784371	3.110004	5.671449
1	0.793018	2.839115	6.063056
1	1.922088	4.169201	5.942406
6	2.823248	2.281315	6.305137
1	2.911500	2.163277	7.385208
6	3.664192	1.698483	5.397538
6	4.562005	0.600656	5.610163
6	5.455796	0.313793	4.577562
1	5.948937	-0.660782	4.592911
1	4.595532	0.582881	3.528041
1	6.107217	1.115142	4.218546
6	4.254228	-0.371480	6.695580
1	3.310941	-0.903677	6.501442
1	5.052418	-1.111697	6.811957
1	4.119685	0.149739	7.654982
6	3.896976	1.762250	2.863741
1	4.957019	1.985366	2.718740

XVIIa

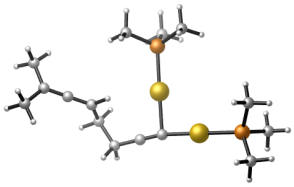


E = -946.498313 h.
G = -946.247983 h.

6	4.141212	2.687120	3.799634
79	3.366337	2.014838	1.466760
15	1.786208	1.403845	-0.139050
6	1.607955	-0.398312	-0.311408
1	1.293271	-0.833110	0.644881
1	0.857850	-0.630020	-1.079517
1	2.569092	-0.840599	-0.599021
6	2.168969	2.005600	-1.811504
1	1.403252	1.659123	-2.518548
1	2.194227	3.101793	-1.814110
1	3.149068	1.631197	-2.129927
6	0.107107	2.015124	0.203303
1	0.108291	3.111411	0.225368

1	-0.583794	1.670117	-0.577756
1	-0.235216	1.644637	1.177014
6	3.547894	4.020096	4.156417
1	4.259063	4.521602	4.830990
1	3.418294	4.672156	3.285185
6	2.257648	3.685589	4.907820
1	1.371291	3.814683	4.264286
1	2.087791	4.312727	5.792357
6	2.429165	2.246734	5.248124
1	1.739425	1.716071	5.902531
6	3.498341	1.673199	4.645143
6	3.866955	0.248025	4.718474
6	5.141543	-0.161446	4.676763
1	5.388567	-1.220859	4.739749
1	5.668730	1.587568	2.745735
1	5.979429	0.531859	4.623804
6	2.735288	-0.724535	4.866965
1	1.993867	-0.601275	4.062502
1	3.097135	-1.759127	4.851056
1	2.198186	-0.573737	5.814610
6	5.096585	2.512514	2.817104
1	5.546264	3.398780	2.364384

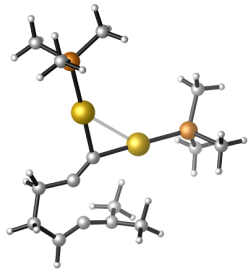
XVIIIa



E = -1542.63441679 h.
G = -1542.298968 h.

6	3.159167	4.839350	2.760532
79	1.818208	3.298238	1.064158
15	1.282029	1.275026	0.055862
6	1.269309	-0.123936	1.221393
1	0.576411	0.080004	2.046735
1	0.957612	-1.041287	0.703245
1	2.274570	-0.270331	1.636243
6	2.423046	0.756841	-1.263643
1	2.098604	-0.206266	-1.680539
1	2.440192	1.510129	-2.060017
1	3.436322	0.652530	-0.857543
6	-0.363630	1.244087	-0.720961
1	-0.425863	2.020574	-1.492873
1	-0.542353	0.261786	-1.179243
1	-1.135375	1.436329	0.033971
6	4.241507	4.390537	3.627210
1	5.155331	4.950855	3.382275
1	3.992098	4.626750	4.672776
6	4.525981	2.883731	3.497611
1	5.430722	2.652065	4.073772
1	4.749384	2.665803	2.440134
6	3.385846	2.023216	3.968006
1	2.402632	2.236034	3.524839
6	3.491613	1.046377	4.834504
6	3.596029	0.060838	5.694360
6	3.415916	0.265617	7.172234
1	2.601478	-0.369727	7.551109
1	4.324966	-0.029649	7.717065
1	3.186060	1.307621	7.422091
6	3.898206	-1.345056	5.256775
1	4.027145	-1.423348	4.170940
1	4.815236	-1.711430	5.741768
1	3.087760	-2.024994	5.559069
6	2.239268	5.232489	2.029588
79	0.711718	6.196848	1.024081
15	-1.030855	7.305151	-0.085521
6	-1.707264	8.744119	0.802669
1	-0.919642	9.489917	0.962883
1	-2.520590	9.196627	0.219463
1	-2.093534	8.430113	1.779732
6	-0.585159	7.959467	-1.725524
1	-0.243451	7.143398	-2.373251
1	-1.455782	8.446341	-2.185266
1	0.225970	8.690916	-1.628026
6	-2.482575	6.250039	-0.399086
1	-3.263485	6.822652	-0.917872
1	-2.192655	5.391564	-1.017356
1	-2.881337	5.875586	0.551348

$TS_{XVIIIa\text{-}XIXa}$

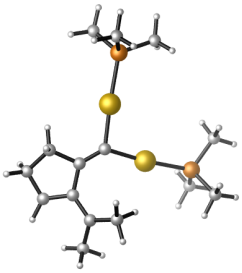


E = -1542.604738 h.
G = -1542.271332 h.

6	3.446007	2.474819	3.077113
79	2.685704	2.944216	0.189533
15	2.951007	3.168704	-2.132192
6	3.447615	1.641524	-2.993227
1	2.683851	0.867480	-2.851632
1	3.570752	1.835583	-4.067470
1	4.396317	1.274329	-2.583546
6	4.219491	4.383348	-2.619031
1	4.288359	4.441866	-3.713782
1	3.961713	5.371467	-2.219592
1	5.193491	4.086429	-2.211883
6	1.453969	3.710013	-3.019879
1	1.117214	4.677989	-2.629310
1	1.662820	3.808009	-4.093997
1	0.651136	2.976964	-2.874813
6	4.937744	2.310523	3.109268
1	5.267651	1.962880	2.122417
1	5.384244	3.304160	3.269760
6	5.372356	1.384801	4.232941
1	6.401862	1.593576	4.550211
1	5.348157	0.329341	3.917563
6	4.390647	1.615602	5.334872
1	4.616982	1.322043	6.360410
6	3.237586	2.186146	5.027580
6	2.008302	2.595062	5.451033
6	1.700789	4.034248	5.584085
1	1.242974	4.345154	4.612512
1	0.944322	4.223478	6.356805
1	2.586334	4.655499	5.755363
6	2.485033	2.758604	2.283983
79	0.480618	3.276588	2.271229
15	-1.792888	3.906693	2.325302
6	-2.941024	2.499734	2.492052
1	-2.663108	1.897762	3.366782
1	-3.970402	2.862421	2.616853
1	-2.888942	1.862480	1.601186
6	-2.159345	4.924603	3.793414

1	-1.544889	5.833254	3.787058
1	-3.221118	5.206186	3.813025
1	-1.924762	4.352766	4.701446
6	-2.464600	4.871458	0.932853
1	-3.525343	5.097732	1.106852
1	-1.908360	5.810906	0.829193
1	-2.365719	4.302257	0.000904
6	0.852705	1.694819	5.304332
1	0.442230	1.882003	4.275587
1	1.111762	0.632438	5.364806
1	0.041953	1.940653	6.002686

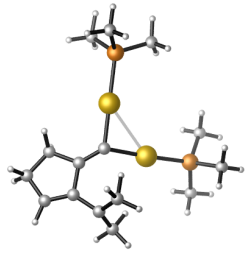
XIXa



E = -1542.619431 h.
G = -1542.284183 h.

6	3.269273	2.514693	3.142835
79	2.678036	2.888671	0.175332
15	2.942819	3.027153	-2.191438
6	3.353091	1.448716	-3.014185
1	2.547816	0.722231	-2.850505
1	3.487477	1.601340	-4.093864
1	4.278569	1.038186	-2.591896
6	4.285196	4.140737	-2.734351
1	4.354450	4.157019	-3.830637
1	4.095986	5.157580	-2.369327
1	5.240776	3.797806	-2.318806
6	1.495141	3.622923	-3.133560
1	1.219315	4.630517	-2.798706
1	1.718248	3.649258	-4.209086
1	0.640895	2.956793	-2.960769
6	4.761143	2.293082	2.887977
1	4.966692	1.224664	2.711594
1	5.106115	2.840416	2.003610
6	5.458899	2.736007	4.181559
1	5.806543	3.785079	4.121041
1	6.338436	2.148531	4.474420
6	4.392273	2.699029	5.199569
1	4.594882	2.731793	6.268692
6	3.148032	2.529561	4.631795
6	2.090659	2.130434	5.473920
6	2.006773	2.520391	6.894439
1	1.030066	3.008397	7.046909
1	1.982720	1.624392	7.532311
1	2.788735	3.204334	7.230670
6	2.327769	2.792790	2.216289
79	0.348101	3.376003	2.321671
15	-1.901040	4.148936	2.227349
6	-3.155371	2.990772	2.874256
1	-2.937471	2.756673	3.924118
1	-4.160053	3.429564	2.803815
1	-3.130861	2.056767	2.299612
6	-2.199910	5.673919	3.186472
1	-1.555149	6.478973	2.813219
1	-3.250264	5.985022	3.103417
1	-1.959339	5.500954	4.242720
6	-2.524774	4.566733	0.562833
1	-3.551846	4.952586	0.620089
1	-1.879076	5.326717	0.105793
1	-2.509810	3.673366	-0.073388
6	0.992233	1.298095	4.969170
1	0.242742	1.982171	4.520170
1	1.303152	0.637400	4.151250
1	0.499107	0.741437	5.774256

$TS_{XIXa-XXa}$

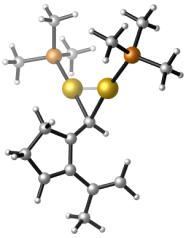


E = -1542.605218 h.
G = -1542.271528 h.

6	3.423845	2.625535	3.334688
79	2.553939	2.635640	0.387737
15	2.700866	2.751971	-1.968779
6	3.199269	1.214664	-2.813514
1	2.474972	0.420026	-2.597795
1	3.245021	1.375978	-3.899113
1	4.184699	0.892300	-2.456048
6	3.887344	3.993220	-2.583460
1	3.898461	3.998758	-3.682034
1	3.603607	4.988500	-2.220391
1	4.893441	3.762168	-2.213316
6	1.133971	3.203535	-2.787856
1	0.775356	4.166210	-2.402822
1	1.277208	3.280644	-3.874310
1	0.374314	2.440395	-2.578912
6	4.844085	3.114055	3.070762
1	5.254998	2.600034	2.192973
1	4.815121	4.183430	2.820754
6	5.662300	2.857057	4.343593
1	6.175056	3.764560	4.692817
1	6.450280	2.102789	4.196373
6	4.654697	2.381862	5.337827
1	4.910716	2.130055	6.365151
6	3.423445	2.255992	4.820444
6	2.141551	1.891647	5.361924
6	1.336767	2.925015	6.046944
1	0.860621	3.532027	5.235835
1	0.521650	2.496373	6.641665
1	1.938300	3.606118	6.658741
6	2.408943	2.534180	2.472429
79	0.404942	3.215360	2.451805
15	-1.722525	4.184233	2.317550
6	-3.107514	2.999090	2.300825
1	-3.087139	2.391103	3.213446
1	-4.063612	3.537511	2.247303
1	-3.020295	2.330982	1.435927
6	-2.105917	5.287775	3.715593
1	-1.359580	6.089338	3.773118
1	-3.103482	5.730753	3.591494
1	-2.078161	4.719183	4.653723
6	-2.001779	5.219213	0.843664
1	-3.015012	5.643028	0.861999
1	-1.268018	6.033964	0.821147
1	-1.879958	4.616275	-0.064652

6	1.479128	0.879630	4.651119
1	1.475008	1.532336	3.568050
1	2.060836	0.015487	4.314665
1	0.445425	0.648617	4.923574

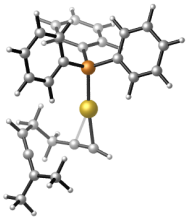
XXa



E = -1542.686421 h.
G = -1542.349009 h.

6	2.640433	2.766963	3.475342
79	2.021355	2.384861	0.577326
15	2.607815	2.220237	-1.688991
6	3.315711	0.612512	-2.170185
1	2.598576	-0.189029	-1.955694
1	3.551026	0.608160	-3.243086
1	4.231706	0.421084	-1.598596
6	3.844365	3.437592	-2.245684
1	4.067022	3.288228	-3.311100
1	3.459471	4.453548	-2.096947
1	4.768195	3.324451	-1.666095
6	1.209656	2.447344	-2.836785
1	0.748217	3.429568	-2.676464
1	1.558950	2.377541	-3.876073
1	0.453325	1.673616	-2.657893
6	3.321544	4.107081	3.330079
1	4.104694	4.019237	2.560961
1	2.629222	4.890385	2.998364
6	3.971530	4.371778	4.693179
1	3.372044	5.071401	5.298390
1	4.976173	4.809795	4.624315
6	3.979755	3.022005	5.323900
1	4.507082	2.819306	6.255224
6	3.259235	2.104010	4.635278
6	3.095707	0.694250	5.029857
6	3.240108	0.381037	6.490157
1	2.569983	0.999821	7.103551
1	3.021198	-0.674184	6.691581
1	4.262599	0.580823	6.842576
6	1.599770	2.308312	2.705896
79	0.015999	3.696003	2.248866
15	-1.806203	5.149038	1.936472
6	-3.439053	4.345706	2.025706
1	-3.574307	3.885737	3.012128
1	-4.235501	5.083883	1.859795
1	-3.509624	3.560619	1.263417
6	-1.915725	6.514332	3.138507
1	-1.000611	7.117508	3.100711
1	-2.780093	7.153071	2.910954
1	-2.022775	6.109520	4.152074
6	-1.809170	5.984408	0.315713
1	-2.687028	6.638310	0.222819
1	-0.898212	6.585626	0.208325
1	-1.828831	5.236076	-0.486176
6	2.884869	-0.280882	4.134371
1	1.222887	1.319437	2.988682
1	2.829967	-0.094873	3.062643
1	2.796137	-1.318641	4.455265

XVb

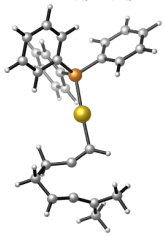


E = -1521.180119 h.
G = -1520.791060 h.

6	4.780962	1.986179	2.607535
79	3.123192	2.491155	0.923609
15	1.570721	2.045663	-0.767541
6	5.115388	0.576767	2.782436
1	5.912278	0.314868	2.073358
1	5.542509	0.476178	3.792670
6	3.943336	-0.390360	2.615803
1	4.343255	-1.412693	2.682946
1	3.533662	-0.295763	1.594731
6	2.830592	-0.217535	3.613810
1	1.980211	-0.895520	3.484421
6	2.816505	0.651069	4.595183
6	2.809884	1.529466	5.570600
6	2.265235	2.917767	5.385254
1	1.480009	3.126408	6.127045
1	3.057894	3.665033	5.544404
1	1.842046	3.069946	4.384439
6	3.357726	1.214850	6.933740
1	3.755549	0.195686	6.996427
1	4.161352	1.918711	7.196722
1	2.575039	1.328769	7.698450
6	4.555855	3.192111	2.501881
1	4.552301	4.260823	2.638992
6	0.062993	1.259440	-0.122286
6	-0.073688	1.071115	1.255483
6	-0.965992	0.857540	-0.983258
6	-1.226790	0.485566	1.771194
1	0.724703	1.390934	1.926964
6	-2.115847	0.276687	-0.463867
1	-0.866477	0.992339	-2.060446
6	-2.246360	0.090160	0.912152
1	-1.325878	0.341688	2.845704
1	-2.914384	-0.033892	-1.135038
1	-3.149791	-0.365169	1.314047
6	1.075695	3.554188	-1.652693
6	1.264339	4.787371	-1.021218
6	0.480322	3.504615	-2.918895
6	0.858937	5.961984	-1.646899
1	1.734153	4.822537	-0.036166
6	0.079504	4.681159	-3.540393
1	0.340247	2.549506	-3.425407
6	0.267731	5.907843	-2.905574
1	1.009927	6.919875	-1.152466
1	-0.379583	4.640890	-4.526397
1	-0.044926	6.826493	-3.398918
6	2.278959	0.911369	-2.001007
6	2.047066	-0.464653	-1.922804
6	3.158531	1.415517	-2.966221
6	2.672900	-1.325855	-2.819853
1	1.370456	-0.867675	-1.169233
6	3.776922	0.549919	-3.860847
1	3.356154	2.486644	-3.024298

6	3.532972	-0.820198	-3.790065
1	2.481313	-2.395714	-2.761443
1	4.453007	0.947242	-4.615733
1	4.016454	-1.495859	-4.493323

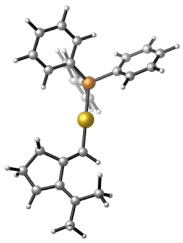
$TS_{XVb\text{-}XVIb}$



E = -1521.161332 h.
G = -1520.773817 h.

6	2.553772	1.622752	3.803023
79	2.720954	1.776146	0.921203
15	1.972697	1.980675	-1.298734
6	1.119113	1.700605	4.145880
1	0.580069	1.956205	3.222727
1	0.769377	0.709915	4.472076
6	0.892952	2.717739	5.254618
1	-0.097298	2.593067	5.709740
1	0.941766	3.745867	4.865589
6	1.983868	2.481249	6.254317
1	1.921719	2.902254	7.258586
6	3.023840	1.773604	5.874933
6	4.117737	0.997786	5.863969
6	5.428610	1.502184	5.379742
1	6.146786	1.459373	6.212548
1	5.836752	0.844501	4.596565
1	5.381215	2.533293	5.015826
6	4.043366	-0.445168	6.234969
1	3.066021	-0.723484	6.640924
1	4.253824	-1.064663	5.349890
1	4.825100	-0.678169	6.971961
6	3.453571	1.587139	2.889349
1	4.530993	1.482998	3.003169
6	3.334717	1.894286	-2.503811
6	4.519904	2.577849	-2.207402
6	3.218480	1.196543	-3.708550
6	5.575953	2.565971	-3.110963
1	4.611907	3.120474	-1.264487
6	4.282129	1.182246	-4.606858
1	2.300900	0.659621	-3.948732
6	5.457204	1.866678	-4.310583
1	6.494979	3.100236	-2.876541
1	4.189219	0.635348	-5.543481
1	6.286871	1.852337	-5.015304
6	0.798111	0.672054	-1.765792
6	-0.216701	0.889866	-2.702629
6	0.963425	-0.596776	-1.200515
6	-1.054249	-0.158397	-3.071560
1	-0.350200	1.875729	-3.148831
6	0.126881	-1.641970	-1.576362
1	1.751721	-0.761900	-0.463610
6	-0.882273	-1.421662	-2.510833
1	-1.843602	0.011938	-3.801482
1	0.258395	-2.627850	-1.133900
1	-1.540247	-2.238759	-2.801592
6	1.123120	3.561933	-1.604012
6	0.244149	4.030827	-0.620942
6	1.306125	4.295056	-2.779130
6	-0.447914	5.220423	-0.814441
1	0.104417	3.460057	0.299709
6	0.615828	5.490010	-2.964665
1	1.986096	3.935365	-3.551454
6	-0.258284	5.952351	-1.985099
1	-1.130558	5.582603	-0.047734
1	0.764097	6.060136	-3.880022
1	-0.792388	6.889422	-2.132977

XVIb

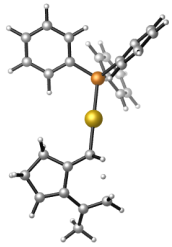


E = -1521.211448 h.
G = -1520.817810 h.

6	2.843085	1.744919	3.827073
79	2.249877	1.176939	0.894395
15	1.719782	1.611104	-1.386789
6	2.570333	3.229714	3.659253
1	3.458233	3.735484	3.249425
1	1.743429	3.417073	2.964611
6	2.291924	3.746199	5.076062
1	1.209666	3.845177	5.285945
1	2.719247	4.728736	5.317342
6	2.799846	2.691649	5.964620
1	2.896405	2.832265	7.039161
6	3.150770	1.551115	5.270307
6	3.843724	0.505392	5.911324
6	4.546113	-0.533255	5.140392
1	5.350708	-0.989487	5.728050
1	3.824601	-1.337411	4.911767
1	4.919655	-0.163954	4.177761
6	3.940352	0.374597	7.377270
1	3.297482	1.040235	7.955586
1	3.709071	-0.667194	7.646589
1	4.989610	0.519724	7.679423
6	2.729226	0.808905	2.866523
1	2.921569	-0.225245	3.166882
6	2.342443	0.336575	-2.531196
6	3.583962	-0.243721	-2.247587
6	1.643725	-0.049131	-3.678417
6	4.124116	-1.193793	-3.107330
1	4.125914	0.051661	-1.346858
6	2.184561	-1.006561	-4.532036
1	0.677102	0.399573	-3.909230
6	3.422555	-1.577138	-4.248280
1	5.090367	-1.642384	-2.883144
1	1.635109	-1.305412	-5.423117
1	3.840935	-2.325868	-4.918850
6	-0.071236	1.719970	-1.711601
6	-0.624807	2.661826	-2.582299
6	-0.902062	0.788872	-1.077534
6	-1.997825	2.670292	-2.814296
1	0.013838	3.389015	-3.083890
6	-2.270900	0.794607	-1.320172
1	-0.470354	0.056586	-0.392348
6	-2.819313	1.737949	-2.186591
1	-2.425131	3.406881	-3.492641
1	-2.912073	0.066244	-0.826768
1	-3.892094	1.747467	-2.371886
6	2.421106	3.187776	-1.975478
6	2.972068	3.337247	-3.250373
6	2.374366	4.285940	-1.108022

6	3.469822	4.574063	-3.652230
1	3.013180	2.489278	-3.934262
6	2.863164	5.521376	-1.517168
1	1.950710	4.168590	-0.108071
6	3.414915	5.664531	-2.788546
1	3.901521	4.684844	-4.645559
1	2.822754	6.372149	-0.839105
1	3.805016	6.629684	-3.107221

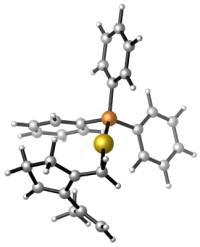
$TS_{XVIb\text{-}XVIIb}$



E = -1521.161932 h.
G = -1520.770987 h.

6	3.420796	2.086099	3.881946
79	2.925633	1.592191	0.923387
15	1.711086	1.564300	-1.118675
6	2.150486	2.881480	3.998274
1	2.156563	3.746756	3.323916
1	1.301306	2.250952	3.689946
6	2.038152	3.253829	5.477146
1	1.045294	3.082933	5.917804
1	2.257895	4.317473	5.664307
6	3.044024	2.404998	6.137036
1	3.150503	2.344530	7.220291
6	3.826988	1.722378	5.246632
6	4.665506	0.587921	5.506330
6	5.505665	0.173800	4.472195
1	5.934467	-0.828383	4.544146
1	4.632835	0.437715	3.425697
1	6.197844	0.902137	4.041129
6	4.341604	-0.282831	6.669912
1	3.354223	-0.754375	6.557439
1	5.090886	-1.069493	6.804080
1	4.295089	0.313766	7.592959
6	3.996032	1.616757	2.712333
1	5.063268	1.774035	2.537101
6	2.749466	1.880305	-2.582128
6	3.768671	2.832473	-2.461205
6	2.534117	1.248068	-3.809198
6	4.555334	3.156316	-3.560629
1	3.940288	3.322527	-1.500422
6	3.329141	1.570553	-4.905605
1	1.743652	0.504850	-3.914207
6	4.336538	2.523536	-4.782597
1	5.344426	3.899783	-3.461747
1	3.159595	1.074828	-5.859936
1	4.955364	2.774211	-5.642597
6	0.422553	2.855671	-1.154467
6	-0.299001	3.092549	0.021747
6	0.128099	3.591360	-2.305330
6	-1.308283	4.048285	0.043092
1	-0.065094	2.522290	0.923338
6	-0.879589	4.551831	-2.277782
1	0.683466	3.415305	-3.226865
6	-1.596453	4.780890	-1.106665
1	-1.865210	4.228450	0.961063
1	-1.104841	5.123531	-3.176486
1	-2.381311	5.535221	-1.088007
6	0.841974	-0.006981	-1.430787
6	1.423424	-1.185541	-0.950697
6	-0.363123	-0.067737	-2.137644
6	0.809715	-2.412240	-1.181036
1	2.358830	-1.137940	-0.390320
6	-0.975655	-1.296816	-2.362243
1	-0.824149	0.845077	-2.516107
6	-0.391524	-2.467129	-1.883493
1	1.264850	-3.325864	-0.802576
1	-1.914574	-1.339500	-2.911502
1	-0.877014	-3.426284	-2.056105

XVIIb

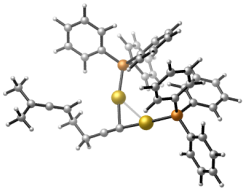


E = -1521.258727 h.
G = -1520.861023 h.

6	4.183280	2.665645	3.603505
79	3.610922	1.752938	1.327774
15	2.003198	1.213761	-0.284084
6	4.022890	4.158681	3.670509
1	4.796159	4.541572	4.353747
1	4.192743	4.641052	2.700741
6	2.627608	4.387654	4.255992
1	1.913613	4.742892	3.494870
1	2.610300	5.138044	5.057732
6	2.230757	3.037455	4.736200
1	1.309191	2.862755	5.289775
6	3.104001	2.060678	4.392430
6	2.922032	0.617969	4.638713
6	3.951259	-0.193715	4.913543
1	3.789901	-1.255703	5.097417
1	5.443690	0.993816	3.073286
1	4.973032	0.169510	5.012319
6	1.512254	0.110274	4.574657
1	1.039209	0.367396	3.613434
1	1.475653	-0.978064	4.701851
1	0.886696	0.560803	5.358755
6	5.189036	2.037808	2.889371
1	5.969037	2.655038	2.439512
6	2.154359	2.133685	-1.841840
6	3.433638	2.481980	-2.287391
6	1.032596	2.469770	-2.606543
6	3.589766	3.155232	-3.493712
1	4.307045	2.223863	-1.685766
6	1.195255	3.146712	-3.810838
1	0.032815	2.200746	-2.264039
6	2.470821	3.489372	-4.252991
1	4.586096	3.427161	-3.837279
1	0.321544	3.409160	-4.404609
1	2.593764	4.021613	-5.194619
6	2.023678	-0.558543	-0.684428
6	1.707706	-1.032572	-1.960281
6	2.307856	-1.463119	0.346046
6	1.678851	-2.403091	-2.201340
1	1.482986	-0.334921	-2.766732
6	2.268314	-2.830471	0.100966
1	2.559387	-1.093601	1.343289
6	1.956022	-3.300003	-1.173414

1	1.436448	-2.769873	-3.197052
1	2.488319	-3.531500	0.903951
1	1.932604	-4.370978	-1.366936
6	0.347432	1.568088	0.385519
6	0.142665	2.812159	0.995840
6	-0.689618	0.634668	0.342990
6	-1.088122	3.114684	1.564133
1	0.951976	3.545273	1.022931
6	-1.921463	0.943114	0.916655
1	-0.539966	-0.335992	-0.129595
6	-2.119580	2.176855	1.528574
1	-1.242251	4.081900	2.039971
1	-2.727359	0.212039	0.885528
1	-3.081209	2.409841	1.982581

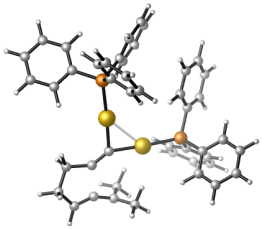
XVIIIb



E = -2692.161160 h.
G = -2691.533164 h.

6	3.096229	4.203374	3.237116
79	2.103293	3.194165	1.039748
15	1.692481	1.824570	-0.796582
6	4.158970	3.579307	4.015766
1	5.103439	4.118035	3.851128
1	3.914755	3.679918	5.084158
6	4.357571	2.090699	3.680111
1	5.181775	1.709994	4.296305
1	4.671543	2.012451	2.626233
6	3.117764	1.272316	3.910243
1	2.247938	1.536795	3.292201
6	3.012134	0.306274	4.788635
6	2.908767	-0.657133	5.673510
6	2.481430	-0.391870	7.089963
1	1.574700	-0.965253	7.333977
1	3.260170	-0.720473	7.794437
1	2.277793	0.669561	7.271429
6	3.213962	-2.089577	5.337623
1	3.496979	-2.218887	4.287087
1	4.033458	-2.467446	5.966965
1	2.340197	-2.725893	5.542657
6	2.175186	4.751329	2.614599
79	0.644300	5.777709	1.683955
15	-1.070107	6.899129	0.534389
6	2.882312	2.085543	-2.146826
6	3.412620	3.367766	-2.327284
6	3.246534	1.052121	-3.014697
6	4.296348	3.614936	-3.372047
1	3.135011	4.171204	-1.641353
6	4.138626	1.303060	-4.052997
1	2.834173	0.051672	-2.881349
6	4.662708	2.580807	-4.230914
1	4.709671	4.612724	-3.507895
1	4.426202	0.495435	-4.723660
1	5.364267	2.771074	-5.041255
6	1.700258	0.039307	-0.448715
6	0.710045	-0.815533	-0.938227
6	2.760449	-0.479721	0.303188
6	0.778692	-2.179913	-0.667463
1	-0.114194	-0.421423	-1.532648
6	2.826781	-1.842509	0.565495
1	3.538876	0.187896	0.677656
6	1.832422	-2.692232	0.083567
1	0.004929	-2.844530	-1.047536
1	3.653501	-2.241451	1.150589
1	1.879802	-3.758841	0.295886
6	0.045682	2.214277	-1.468007
6	-0.201460	2.266012	-2.842206
6	-0.996628	2.456675	-0.563790
6	-1.480711	2.564679	-3.306563
1	0.601595	2.076077	-3.554629
6	-2.273710	2.742283	-1.032975
1	-0.803554	2.433449	0.511537
6	-2.514120	2.802397	-2.404801
1	-1.668017	2.611785	-4.377897
1	-3.080689	2.932223	-0.325415
1	-3.511902	3.041535	-2.769973
6	-0.680248	7.075186	-1.237351
6	-0.158483	5.959713	-1.903772
6	-0.908400	8.259615	-1.941425
6	0.122553	6.027014	-3.262930
1	0.017756	5.030447	-1.354523
6	-0.612508	8.325746	-3.300984
1	-1.318963	9.131738	-1.432501
6	-0.099315	7.213118	-3.960837
1	0.516346	5.151590	-3.778827
1	-0.788367	9.251910	-3.845433
1	0.129006	7.268626	-5.023849
6	-2.654909	6.006320	0.606490
6	-3.578173	6.055014	-0.442388
6	-2.954109	5.281299	1.765014
6	-4.794087	5.388083	-0.326447
1	-3.347820	6.616185	-1.348992
6	-4.171837	4.618487	1.877624
1	-2.228499	5.237443	2.579570
6	-5.090702	4.671497	0.831102
1	-5.512803	5.428685	-1.143251
1	-4.402874	4.056520	2.780819
1	-6.043229	4.151450	0.918210
6	-1.390706	8.581409	1.148358
6	-0.289633	9.372025	1.497443
6	-2.681530	9.107018	1.241363
6	-0.479659	10.679674	1.929089
1	0.718702	8.959206	1.426974
6	-2.866517	10.414634	1.682520
1	-3.545204	8.499808	0.970836
6	-1.769055	11.199436	2.024485
1	0.379684	11.290812	2.199130
1	-3.873618	10.820560	1.759214
1	-1.918153	12.220704	2.370864

$TS_{XVIIIb\text{-}XIXb}$

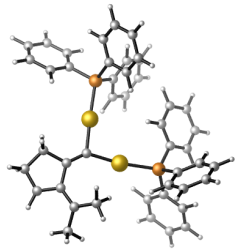


E = -2692.128723 h.
G = -2691.498822 h.

6	3.490281	3.036659	3.114394
79	2.605649	3.166497	0.244875
15	2.851973	3.309818	-2.092832
6	4.988925	3.091497	3.100653
1	5.339180	2.706934	2.134390

1	5.286687	4.149822	3.156649
6	5.590681	2.342477	4.277846
1	6.588874	2.723961	4.527385
1	5.710525	1.270490	4.053720
6	4.625876	2.527947	5.402963
1	4.927801	2.352795	6.436177
6	3.393397	2.902403	5.108156
6	2.126282	3.174475	5.523241
6	1.623721	4.564347	5.543506
1	1.145879	4.729987	4.547772
1	0.834465	4.707968	6.292739
1	2.413295	5.313468	5.667273
6	2.469652	3.107912	2.350459
79	0.412234	3.327649	2.323590
15	-1.934640	3.576030	2.161483
6	1.106513	2.114697	5.465688
1	0.698262	2.145412	4.420150
1	1.507308	1.108426	5.628857
1	0.257009	2.315269	6.131322
6	4.472695	4.004762	-2.554127
6	5.588477	3.613222	-1.804984
6	4.634156	4.883696	-3.628384
6	6.852247	4.090815	-2.131462
1	5.461615	2.928713	-0.963451
6	5.901197	5.364662	-3.947487
1	3.773104	5.194749	-4.220082
6	7.007737	4.970903	-3.200602
1	7.716388	3.783850	-1.544807
1	6.021680	6.053239	-4.781900
1	7.996249	5.352035	-3.451165
6	2.738882	1.697289	-2.932086
6	3.543292	1.369261	-4.026851
6	1.797334	0.774774	-2.461234
6	3.404577	0.128968	-4.643411
1	4.278450	2.081119	-4.402498
6	1.658059	-0.459980	-3.084725
1	1.178087	1.025467	-1.597368
6	2.464196	-0.783972	-4.174086
1	4.033888	-0.124293	-5.494818
1	0.926055	-1.174704	-2.712589
1	2.359877	-1.754285	-4.656746
6	1.610718	4.384671	-2.881677
6	1.139818	4.151664	-4.177477
6	1.169153	5.508584	-2.174089
6	0.239445	5.040430	-4.759407
1	1.479581	3.280290	-4.737903
6	0.272887	6.395250	-2.760899
1	1.528840	5.685473	-1.158127
6	-0.191786	6.160782	-4.053565
1	-0.124052	4.856901	-5.769006
1	-0.072631	7.264100	-2.203211
1	-0.898940	6.852295	-4.509045
6	-2.618275	4.675432	3.442084
6	-3.857002	4.441328	4.045403
6	-1.879136	5.811241	3.793435
6	-4.346118	5.333790	4.995249
1	-4.444456	3.563479	3.775060
6	-2.374148	6.702600	4.738559
1	-0.913500	5.995732	3.317670
6	-3.606794	6.461757	5.341768
1	-5.310023	5.147429	5.465809
1	-1.794942	7.584457	5.007159
1	-3.992475	7.156917	6.085609
6	-2.466682	4.265458	0.562052
6	-3.467664	5.233604	0.454892
6	-1.870356	3.750542	-0.595437
6	-3.866813	5.682179	-0.802041
1	-3.941112	5.638670	1.349348
6	-2.282279	4.190791	-1.847304
1	-1.080559	2.999186	-0.510616
6	-3.279296	5.159951	-1.950354
1	-4.644032	6.440276	-0.882466
1	-1.814785	3.788562	-2.745614
1	-3.594342	5.512675	-2.931431
6	-2.831229	1.997582	2.321126
6	-3.956436	1.704266	1.546234
6	-2.380005	1.071239	3.268230
6	-4.618608	0.491433	1.714770
1	-4.318834	2.422590	0.810514
6	-3.048815	-0.135673	3.437787
1	-1.500591	1.300116	3.873595
6	-4.165549	-0.427509	2.657292
1	-5.492716	0.263883	1.107061
1	-2.691644	-0.853307	4.174366
1	-4.683255	-1.376762	2.784496

XIXb



E = -2692.146121 h.
G = -2691.514014 h.

6	3.495749	3.035856	3.171613
79	2.671169	3.205455	0.247993
15	2.792731	3.312548	-2.138765
6	4.967452	2.886428	2.771755
1	5.192950	1.828412	2.563100
1	5.192854	3.447982	1.857500
6	5.783908	3.362112	3.980190
1	6.140723	4.400721	3.849428
1	6.678537	2.769573	4.212740
6	4.815632	3.370050	5.091742
1	5.115365	3.456579	6.134796
6	3.524677	3.159408	4.666759
6	2.541113	2.893553	5.644055
6	2.589637	3.475664	6.998775
1	1.649555	4.030703	7.154328
1	2.578883	2.676495	7.754752
1	3.422323	4.159546	7.176507
6	2.464095	3.153573	2.313190
79	0.421806	3.418572	2.398494
15	-1.935518	3.691038	2.162742
6	1.385247	2.053821	5.336797
1	0.688870	2.690378	4.741296
1	1.630051	1.222205	4.664142
1	0.860791	1.708047	6.233875
6	-2.877166	2.161923	2.488199
6	-2.441266	1.341327	3.535170
6	-4.014126	1.802833	1.759184
6	-3.140845	0.183409	3.856370
1	-1.547481	1.613679	4.100173
6	-4.707344	0.638355	2.078471
1	-4.362823	2.432055	0.940263
6	-4.273717	-0.169201	3.126210
1	-2.797905	-0.449116	4.673442
1	-5.590766	0.363200	1.504720
1	-4.819211	-1.078712	3.372560

6	-2.652556	4.948902	3.273218
6	-3.905444	4.805319	3.875316
6	-1.902205	6.107905	3.505014
6	-4.399914	5.811841	4.700902
1	-4.498973	3.907904	3.699637
6	-2.403103	7.113707	4.323915
1	-0.919877	6.218007	3.040929
6	-3.651294	6.964045	4.924891
1	-5.375227	5.693447	5.170232
1	-1.815306	8.012759	4.501206
1	-4.040234	7.746964	5.573820
6	-2.393852	4.211636	0.475784
6	-3.512901	5.005306	0.206225
6	-1.590258	3.769693	-0.581282
6	-3.823424	5.347647	-1.106933
1	-4.146917	5.355368	1.021579
6	-1.905524	4.110341	-1.892063
1	-0.707868	3.160624	-0.367826
6	-3.021032	4.902299	-2.154561
1	-4.695390	5.966329	-1.312417
1	-1.271806	3.769875	-2.711624
1	-3.260689	5.178026	-3.180658
6	1.701213	4.574317	-2.878572
6	1.439606	5.729714	-2.133201
6	1.130864	4.428139	-4.147283
6	0.621412	6.728084	-2.651937
1	1.872419	5.839685	-1.136739
6	0.308099	5.427018	-4.660903
1	1.330238	3.533878	-4.738829
6	0.052981	6.575334	-3.914451
1	0.417387	7.621805	-2.064715
1	-0.135213	5.306813	-5.648193
1	-0.596097	7.351634	-4.316556
6	4.473707	3.689272	-2.739327
6	4.724069	4.551686	-3.809231
6	5.544609	3.061564	-2.091143
6	6.033275	4.783885	-4.224129
1	3.898346	5.045139	-4.322183
6	6.849053	3.288633	-2.514847
1	5.349766	2.391017	-1.251003
6	7.093766	4.153368	-3.579917
1	6.223544	5.460480	-5.055572
1	7.677017	2.795715	-2.008071
1	8.115929	4.338439	-3.906036
6	2.331283	1.743144	-2.947758
6	2.965976	1.268890	-4.099225
6	1.278872	1.010055	-2.386524
6	2.548577	0.075193	-4.681815
1	3.787247	1.831235	-4.544633
6	0.860819	-0.178155	-2.975142
1	0.790121	1.373480	-1.479976
6	1.497788	-0.647057	-4.122003
1	3.047010	-0.291840	-5.577478
1	0.042506	-0.742999	-2.531918
1	1.175426	-1.581266	-4.578864

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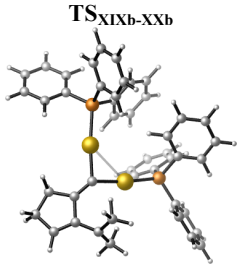

E = -2692.133957 h.

G = -2691.506124 h.

6	3.619889	2.903095	3.503689
79	2.811822	2.678494	0.529559
15	2.748801	2.742811	-1.838418
6	5.032223	3.414472	3.248294
1	5.515835	2.788224	2.487546
1	4.982297	4.428677	2.830104
6	5.777775	3.387391	4.590601
1	6.185015	4.374501	4.852919
1	6.635770	2.698594	4.586757
6	4.745897	2.949154	5.577130
1	4.956797	2.828690	6.637962
6	3.557206	2.686905	5.013193
6	2.267231	2.300737	5.526548
6	1.370268	3.345244	6.061927
1	0.919891	3.846702	5.167328
1	0.537662	2.930983	6.642979
1	1.894658	4.115660	6.637712
6	2.648856	2.686832	2.612386
79	0.613130	3.258683	2.464522
6	1.700538	1.187309	4.894666
1	1.714283	1.748971	3.745732
1	2.343948	0.334944	4.655235
1	0.668159	0.922117	5.139627
15	-1.571623	4.011066	2.049867
6	-2.607214	4.038184	3.550030
6	-2.565183	2.914094	4.384712
6	-3.420237	5.121230	3.889791
6	-3.335082	2.872276	5.540358
1	-1.926563	2.067857	4.122106
6	-4.180441	5.080187	5.056854
1	-3.461926	6.001108	3.248430
6	-4.139572	3.959222	5.879777
1	-3.303091	1.993482	6.182112
1	-4.806791	5.930508	5.320854
1	-4.734917	3.931747	6.790734
6	-2.426532	2.919162	0.864813
6	-1.688672	2.416286	-0.214225
6	-3.775035	2.578254	0.999976
6	-2.293918	1.576853	-1.142903
1	-0.633922	2.684401	-0.325366
6	-4.375765	1.736146	0.067747
1	-4.359376	2.966675	1.834475
6	-3.636795	1.233268	-0.999188
1	-1.714015	1.179110	-1.975028
1	-5.425736	1.470915	0.178619
1	-4.107313	0.568082	-1.721173
6	-1.651930	5.685594	1.338609
6	-0.625337	6.589827	1.629475
6	-2.727630	6.088904	0.540975
6	-0.680234	7.889805	1.135443
1	0.221521	6.272997	2.241355
6	-2.777938	7.388687	0.047148
1	-3.530095	5.388279	0.307559
6	-1.756382	8.288395	0.345055
1	0.120650	8.590763	1.363714
1	-3.617741	7.698836	-0.572346
1	-1.797962	9.304746	-0.042934
6	4.186971	3.547986	-2.611997
6	5.439781	3.356206	-2.019562
6	4.078994	4.320604	-3.772364
6	6.575260	3.923174	-2.588152
1	5.520242	2.762134	-1.107062
6	5.217446	4.890365	-4.334789
1	3.106417	4.475499	-4.241062
6	6.463114	4.691745	-3.744350

1	7.547832	3.772380	-2.122755
1	5.130951	5.491665	-5.238054
1	7.350918	5.141442	-4.185853
6	2.571107	1.118009	-2.640343
6	3.083434	0.849586	-3.912819
6	1.866880	0.123415	-1.952201
6	2.891596	-0.402854	-4.488499
1	3.633646	1.617715	-4.456543
6	1.671377	-1.124386	-2.534315
1	1.476704	0.328639	-0.952839
6	2.187553	-1.388197	-3.801148
1	3.296294	-0.609127	-5.477809
1	1.125582	-1.896064	-1.994235
1	2.043817	-2.367921	-4.253843
6	1.289787	3.714198	-2.348434
6	0.432443	3.318879	-3.377721
6	1.027587	4.896661	-1.643894
6	-0.682613	4.094475	-3.691184
1	0.630097	2.402629	-3.934892
6	-0.080121	5.671516	-1.966182
1	1.696964	5.208792	-0.838500
6	-0.941345	5.265314	-2.984600
1	-1.351141	3.777596	-4.489953
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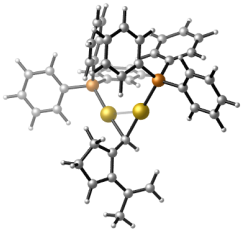
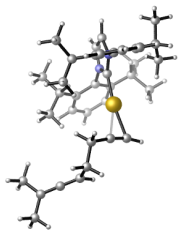
XXb



E = -2692.214091 h.
G = -2691.581188 h.

6	2.817425	2.521829	3.589199
79	1.925450	2.164266	0.759362
15	2.209273	2.204361	-1.575997
6	3.590490	3.786576	3.302557
1	4.322528	3.568977	2.508995
1	2.948501	4.598511	2.938328
6	4.333664	4.099984	4.605325
1	3.817611	4.881450	5.186869
1	5.360152	4.458785	4.453035
6	4.283921	2.800971	5.332106
1	4.847198	2.625504	6.247564
6	3.459686	1.892783	4.754443
6	3.218400	0.532954	5.267750
6	3.441509	0.319254	6.735991
1	2.836283	1.009955	7.340083
1	3.192352	-0.707565	7.028123
1	4.491481	0.497304	7.010605
6	1.695265	2.097580	2.918560
79	0.177629	3.583748	2.529317
15	-1.482976	5.151634	1.957702
6	2.870619	-0.486159	4.469402
1	1.270881	1.154793	3.277755
1	2.751571	-0.378418	3.392313
1	2.727148	-1.486171	4.878314
6	-1.698143	6.563150	3.083358
6	-1.565175	6.334301	4.456953
6	-2.022464	7.841241	2.618574
6	-1.760938	7.374372	5.358909
1	-1.305306	5.336850	4.816281
6	-2.210413	8.880197	3.525274
1	-2.131206	8.026178	1.549455
6	-2.080258	8.647489	4.892216
1	-1.656607	7.192613	6.427106
1	-2.460494	9.875476	3.162127
1	-2.225965	9.462766	5.598725
6	-1.040594	5.845797	0.328382
6	0.309125	6.131655	0.083591
6	-1.985980	6.064579	-0.677135
6	0.706957	6.627873	-1.152788
1	1.052855	5.953838	0.864829
6	-1.582685	6.558754	-1.915840
1	-3.039258	5.847261	-0.497452
6	-0.239659	6.835320	-2.155381
1	1.759929	6.838812	-1.341892
1	-2.323222	6.720811	-2.697389
1	0.074355	7.211256	-3.127934
6	-3.129911	4.406878	1.738715
6	-4.307165	5.067355	2.097201
6	-3.196771	3.138942	1.147536
6	-5.540183	4.463321	1.863035
1	-4.264778	6.053551	2.559638
6	-4.430122	2.545021	0.906730
1	-2.276959	2.617983	0.871063
6	-5.602435	3.207403	1.266262
1	-6.455307	4.980454	2.146207
1	-4.476548	1.560924	0.443559
1	-6.568450	2.738784	1.085538
6	2.921000	3.785056	-2.139940
6	3.887263	4.399944	-1.335504
6	2.543974	4.381358	-3.346775
6	4.477129	5.592903	-1.740091
1	4.178358	3.938944	-0.389257
6	3.135349	5.576415	-3.747175
1	1.786737	3.913249	-3.976701
6	4.100376	6.181753	-2.945788
1	5.229843	6.065685	-1.111663
1	2.838588	6.036343	-4.688302
1	4.559605	7.117156	-3.261002
6	0.617118	2.045255	-2.450951
6	-0.426023	2.899550	-2.068468
6	0.406663	1.105116	-3.461059
6	-1.662931	2.812692	-2.695176
1	-0.262268	3.649272	-1.288676
6	-0.839380	1.015712	-4.078705
1	1.213264	0.440584	-3.769717
6	-1.872718	1.864748	-3.696230
1	-2.466709	3.486767	-2.400179
1	-0.998390	0.277865	-4.863163
1	-2.845005	1.790541	-4.180326
6	3.287672	0.892199	-2.228782
6	3.378188	-0.306549	-1.514096
6	3.989435	1.041096	-3.429241
6	4.162236	-1.349223	-1.997072
1	2.834568	-0.417422	-0.573845
6	4.776579	-0.002252	-3.905364
1	3.922954	1.972058	-3.993045
6	4.862037	-1.195320	-3.190929
1	4.231868	-2.280122	-1.437242
1	5.324564	0.117174	-4.838310
1	5.482011	-2.008211	-3.565215

XVc



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G = -1643.956359 h.

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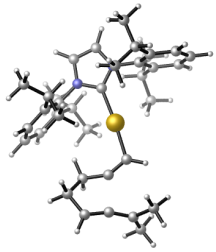
6	3.481038	2.901139	3.711560
1	3.939035	2.205670	4.425885
1	2.725410	3.484694	4.258046
6	4.526899	3.814682	3.134326
1	4.166208	4.636636	2.505375
6	5.814826	3.677146	3.331949
6	7.102774	3.550733	3.546793
6	7.986591	2.721421	2.658581
1	8.775259	3.345918	2.213168
1	8.495197	1.939949	3.242507
1	7.429415	2.238294	1.847764
6	7.788275	4.235765	4.695644
1	7.091501	4.818959	5.308051
1	8.285712	3.497999	5.342546
1	8.573472	4.912329	4.326386
6	1.418380	3.731745	1.025337
1	0.919002	4.605195	0.639969
6	1.298053	0.691495	-1.933984
7	1.992354	0.770288	-3.089691
7	0.547822	-0.427394	-2.041154
6	1.691206	-0.300064	-3.915337
1	2.146445	-0.407436	-4.892034
6	0.783873	-1.058138	-3.251422
1	0.294630	-1.988577	-3.511386
6	-0.211306	-0.984608	-0.953338
6	0.491054	-1.790814	-0.042620
6	-1.580001	-0.697145	-0.828141
6	-0.216345	-2.307266	1.044537
6	-2.235734	-1.244452	0.278265
6	-1.567704	-2.033735	1.206669
1	0.302564	-2.933031	1.770368
1	-3.299692	-1.042822	0.405886
1	-2.107133	-2.442542	2.059484
6	2.934836	1.812599	-3.398069
6	4.220551	1.736520	-2.835553
6	2.518360	2.863944	-4.225756
6	5.117199	2.754028	-3.161753
6	3.453448	3.862079	-4.510752
6	4.739730	3.804138	-3.991611
1	6.127486	2.727273	-2.756286
1	5.456005	4.588982	-4.229321
6	-2.422538	0.085757	-1.821830
1	-3.349030	0.323406	-1.276005
6	1.103759	2.970143	-4.755726
1	0.571848	2.035155	-4.525201
6	1.963138	-2.116427	-0.204433
1	2.331237	-1.657159	-1.134786
6	4.637521	0.596210	-1.928567
1	3.727959	0.162220	-1.488297
6	2.774617	2.059848	2.634693
1	2.080069	1.345331	3.099513
1	3.520136	1.469009	2.082393
6	-2.825180	-0.798372	-3.002567
1	-1.956080	-1.065324	-3.620493
1	-3.298301	-1.729441	-2.663094
1	-3.539594	-0.269729	-3.648369
6	-1.859519	1.418125	-2.311519
1	-1.455522	2.023256	-1.487115
1	-1.068187	1.289595	-3.063208
1	-2.663125	1.995196	-2.789550
6	2.183274	-3.621963	-0.332194
1	1.891153	-4.153689	0.584213
1	1.602407	-4.042487	-1.164655
1	3.244704	-3.836904	-0.516957
6	2.787051	-1.536630	0.941752
1	2.487433	-1.964972	1.909137
1	3.854455	-1.756612	0.796584
1	2.665993	-0.443868	1.006540
6	5.513781	1.057896	-0.768549
1	5.675323	0.231260	-0.062881
1	6.506205	1.389000	-1.105719
1	5.051959	1.891491	-0.217577
6	5.325549	-0.508716	-2.728173
1	4.682950	-0.880970	-3.538253
1	6.258973	-0.140802	-3.179456
1	5.575513	-1.358708	-2.076724
6	1.070674	3.144832	-6.270786
1	0.032672	3.148930	-6.629207
1	1.529253	4.093453	-6.582309
1	1.602681	2.329934	-6.780709
6	0.354352	4.101784	-4.052837
1	-0.688135	4.144719	-4.398161
1	0.345505	3.961965	-2.961113
1	0.816824	5.077146	-4.262751
1	3.165758	4.700289	-5.144785

$TS_{XVc\text{-}XVIc}$

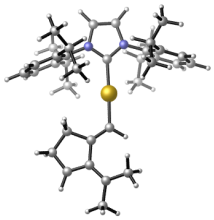


E = -1644.620179 h.
G = -1643.940849 h.

6	2.919465	2.719300	2.075913
79	2.846377	1.784931	-0.599171
6	1.028698	2.455096	3.627630
1	0.587620	1.787230	4.378294
1	0.205104	2.808197	2.986784
6	1.732375	3.612437	4.269940
1	1.277988	4.154341	5.100190
6	2.901729	3.963633	3.782420
6	4.133937	4.475330	3.641722
6	4.421304	5.563817	2.672301
1	4.767023	6.444077	3.235194
1	5.250992	5.286886	2.003826
1	3.545257	5.853383	2.083300
6	5.295473	3.901264	4.381261
1	4.991819	3.150502	5.117338
1	5.998060	3.442546	3.669162
1	5.845533	4.707216	4.887709
6	3.461432	3.055143	0.959948
1	4.115467	3.898347	0.747552
6	2.111760	0.508674	-2.038175
7	2.394739	0.388790	-3.355902
7	1.169960	-0.431646	-1.793535

6	1.655950	-0.639008	-3.924389
1	1.767654	-0.909591	-4.966769
6	0.875403	-1.149715	-2.940955
1	0.146177	-1.950351	-2.939716
6	0.612597	-0.675262	-0.490527
6	1.277131	-1.575756	0.355539
6	-0.539585	0.025319	-0.106035
6	0.744412	-1.771534	1.631654
6	-1.032586	-0.206883	1.180103
6	-0.399137	-1.095856	2.040385
1	1.235637	-2.463838	2.315623
1	-1.925332	0.322909	1.512778
1	-0.800714	-1.261866	3.039150
6	3.442427	1.120177	-4.018830
6	4.752381	0.637358	-3.865864
6	3.134750	2.268183	-4.769174
6	5.782791	1.343931	-4.489706
6	4.206216	2.929162	-5.375909
6	5.513980	2.480524	-5.238596
1	6.808991	0.991519	-4.386836
1	6.326890	3.019732	-5.722446
6	-1.217633	1.034096	-1.006664
1	-0.699473	1.037451	-1.976534
6	1.740959	2.816023	-5.030822
1	1.908173	3.827378	-5.433769
6	2.538949	-2.303998	-0.054998
1	2.789069	-2.013390	-1.085983
6	5.082561	-0.612800	-3.075687
1	4.150342	-1.031709	-2.670898
6	2.087599	1.737406	2.806968
1	1.649558	1.058625	2.060086
1	2.730440	1.132739	3.465108
6	0.834622	2.980785	-3.813385
1	0.448318	2.018956	-3.450300
1	1.348078	3.481060	-2.980079
1	-0.034605	3.594609	-4.087589
6	1.032206	2.023373	-6.129709
1	1.655365	1.940325	-7.030258
1	0.778231	1.007307	-5.796032
1	0.094523	2.521851	-6.411783
6	5.992706	-0.299282	-1.890718
1	6.181358	-1.208498	-1.302456
1	6.965970	0.088753	-2.224294
1	5.540995	0.450389	-1.222548
6	5.702807	-1.678733	-3.976143
1	5.040539	-1.929589	-4.816594
1	6.662965	-1.343037	-4.392896
1	5.891862	-2.598736	-3.406277
6	2.334735	-3.816612	-0.043102
1	2.120235	-4.185210	0.970099
1	1.500413	-4.114012	-0.693306
1	3.239925	-4.328203	-0.397347
6	3.712564	-1.900703	0.835055
1	3.534767	-2.186243	1.882105
1	4.635535	-2.398505	0.506342
1	3.881690	-0.812656	0.807497
6	-1.104809	2.440287	-0.418329
1	-1.522568	3.184421	-1.111082
1	-1.660199	2.518273	0.528077
1	-0.055468	2.711285	-0.216283
6	-2.674039	0.665663	-1.274437
1	-2.760431	-0.340239	-1.707976
1	-3.274084	0.689101	-0.354050
1	-3.122636	1.378236	-1.979841
1	3.998824	3.820085	-5.969214

XVIc

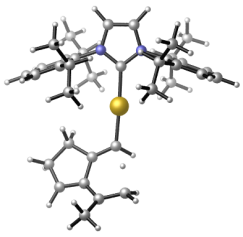


E = -1644.671840 h.
G = -1643.989028 h.

6	3.326997	2.971646	2.182384
79	2.957527	1.670642	-0.526860
6	2.376951	2.228653	4.291190
1	2.838461	1.319862	4.721627
1	1.454225	2.376914	4.869100
6	3.328354	3.329763	4.494456
1	3.548279	3.735442	5.479832
6	3.855479	3.790830	3.304920
6	4.618553	4.974810	3.279753
6	4.850871	5.706904	2.024517
1	5.060156	6.766079	2.213605
1	5.750426	5.287175	1.540934
1	4.029370	5.586744	1.308167
6	5.225592	5.574158	4.483664
1	5.185563	4.963288	5.387292
1	6.278042	5.804557	4.257175
1	4.756061	6.551591	4.676005
6	3.780424	2.888693	0.915316
1	4.630887	3.531093	0.664453
6	2.046799	0.444237	-1.942824
7	2.325342	0.311417	-3.260962
7	0.998789	-0.388753	-1.733138
6	1.467088	-0.590964	-3.869283
1	1.542683	-0.826246	-4.923706
6	0.628653	-1.035593	-2.901722
1	-0.191943	-1.741667	-2.925802
6	0.384127	-0.592302	-0.451187
6	0.900579	-1.595077	0.382199
6	-0.694021	0.227503	-0.083800
6	0.292068	-1.771613	1.627217
6	-1.262517	0.013305	1.173279
6	-0.777614	-0.976686	2.019588
1	0.664633	-2.545923	2.298312
1	-2.099202	0.632912	1.495218
1	-1.239541	-1.129940	2.994038
6	3.384839	1.014713	-3.926156
6	4.654247	0.420937	-3.969202
6	3.106756	2.269464	-4.486607
6	5.673260	1.133535	-4.604209
6	4.159419	2.940025	-5.112386
6	5.429475	2.379465	-5.170296
1	6.674715	0.706416	-4.655499
1	6.237809	2.916949	-5.663972
6	-1.209394	1.336830	-0.976807
1	-0.752888	1.219327	-1.971008
6	1.733273	2.903847	-4.424745
1	1.055519	2.217288	-3.896191
6	2.067079	-2.474213	-0.018083
1	2.423017	-2.156833	-1.009863
6	4.942327	-0.925191	-3.337243
1	3.994909	-1.348092	-2.969792
6	2.197793	2.139076	2.770563
1	1.220211	2.557231	2.482772
1	2.221799	1.106709	2.401619
6	5.517874	-1.909904	-4.351098

1	4.850435	-2.030618	-5.215421
1	6.497609	-1.580688	-4.725059
1	5.656386	-2.896911	-3.889164
6	5.868505	-0.769332	-2.132471
1	6.041606	-1.742323	-1.651853
1	6.846935	-0.366916	-2.432473
1	5.437977	-0.086907	-1.383244
6	1.163746	3.119474	-5.824563
1	0.150268	3.539493	-5.766439
1	1.781670	3.818942	-6.405467
1	1.108465	2.175607	-6.384830
6	1.765913	4.210510	-3.635475
1	0.756018	4.636106	-3.554524
1	2.151892	4.053730	-2.616598
1	2.404146	4.959706	-4.125736
6	3.235336	-2.322950	0.953271
1	2.954952	-2.624725	1.972459
1	4.076987	-2.956324	0.640801
1	3.592019	-1.282471	0.993905
6	1.632254	-3.933609	-0.131705
1	1.286026	-4.323172	0.836292
1	0.813023	-4.053905	-0.854209
1	2.471316	-4.560851	-0.462165
6	-2.722741	1.274192	-1.162320
1	-3.048542	2.038294	-1.880904
1	-3.044857	0.294557	-1.540406
1	-3.257431	1.463694	-0.221222
6	-0.785273	2.700594	-0.430772
1	-1.240748	2.888254	0.553223
1	0.309042	2.765785	-0.314010
1	-1.106784	3.504908	-1.107362
1	3.979455	3.917478	-5.560655

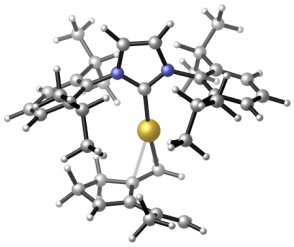
$TS_{XVIc\text{-}XVIIc}$



E = -1644.622911 h.
G = -1643.943691 h.

6	3.542501	2.586492	2.358572
79	3.135370	1.543982	-0.448720
6	2.407404	1.900944	4.378095
1	2.890975	1.162837	5.037936
1	1.362207	1.949585	4.717357
6	3.051933	3.217027	4.526086
1	3.030137	3.786283	5.455488
6	3.686061	3.628641	3.386555
6	4.129525	4.952619	3.058240
6	4.911177	5.083360	1.910434
1	5.028893	6.084912	1.490025
1	5.816690	4.477130	1.827828
1	4.250253	4.133829	1.143203
6	3.450274	6.114088	3.697054
1	3.434077	5.999557	4.790645
1	3.951831	7.056239	3.453327
1	2.399172	6.187116	3.380027
6	4.056447	2.627152	1.071870
1	5.131485	2.755392	0.921398
6	2.118852	0.494800	-1.927095
7	2.373579	0.401763	-3.251878
7	0.999657	-0.244968	-1.742696
6	1.427274	-0.383292	-3.891906
1	1.472244	-0.570685	-4.957465
6	0.554697	-0.788890	-2.937258
1	-0.331561	-1.409247	-2.982955
6	0.356544	-0.404488	-0.469136
6	0.689134	-1.520093	0.313690
6	-0.552345	0.579789	-0.055812
6	0.066019	-1.637461	1.557696
6	-1.148483	0.414783	1.196861
6	-0.844271	-0.681855	1.994356
1	0.302121	-2.487970	2.196491
1	-1.865804	1.155878	1.549767
1	-1.322033	-0.794631	2.966709
6	3.474096	1.053548	-3.902525
6	4.705219	0.386463	-3.963818
6	3.267525	2.334093	-4.434371
6	5.760888	1.047358	-4.595180
6	4.355382	2.952329	-5.053977
6	5.588186	2.315432	-5.136150
1	6.732875	0.558489	-4.663072
1	6.423057	2.813920	-5.626608
6	-0.898551	1.784587	-0.905988
1	-0.286410	1.756976	-1.820732
6	1.942570	3.058218	-4.313461
1	1.196650	2.357560	-3.907778
6	1.727514	-2.532199	-0.125400
1	1.928625	-2.379740	-1.196342
6	4.917987	-0.986924	-3.363813
1	3.965616	-1.330146	-2.931944
6	2.572621	1.569590	2.894789
1	1.612208	1.657323	2.360610
1	2.930893	0.548130	2.712450
6	1.427625	3.538786	-5.666923
1	0.434281	3.994004	-5.554784
1	2.088950	4.298706	-6.106162
1	1.343135	2.711290	-6.384347
6	2.060218	4.222873	-3.331132
1	1.092212	4.730834	-3.218883
1	2.387641	3.878884	-2.337116
1	2.788434	4.966647	-3.686496
6	5.326517	-1.998150	-4.431522
1	4.573448	-2.065388	-5.229017
1	6.284291	-1.725175	-4.896705
1	5.444505	-2.997342	-3.990396
6	5.941699	-0.932433	-2.232282
1	6.047949	-1.918531	-1.758894
1	6.932114	-0.632213	-2.603905
1	5.640700	-0.211206	-1.456826
6	1.253587	-3.971769	0.050010
1	1.124749	-4.232684	1.109803
1	0.297379	-4.149798	-0.459848
1	1.994443	-4.667110	-0.366821
6	3.039304	-2.300594	0.624901
1	2.907329	-2.468641	1.704388
1	3.815374	-2.993041	0.269431
1	3.408421	-1.271289	0.487327
6	-2.365133	1.743149	-1.328721
1	-2.597545	0.824306	-1.885073
1	-3.032849	1.784014	-0.456049
1	-2.606537	2.599393	-1.973131
6	-0.571328	3.087516	-0.179588
1	-0.795384	3.951101	-0.820625
1	-1.164811	3.196038	0.739585
1	0.494150	3.135013	0.095536
1	4.236152	3.950257	-5.475816

XVIIc



E = -1644.724054 h.
G = -1644.038190 h.

6	4.102733	2.309516	2.048818
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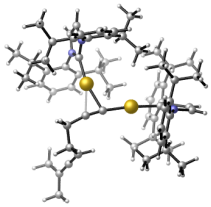
6	2.200248	2.169761	3.517198
1	2.020842	2.201907	4.599661
1	1.317869	1.672385	3.075242
6	2.371401	3.523108	2.924369
1	1.675910	4.337167	3.123295
6	3.445688	3.625673	2.104395
6	3.809587	4.828502	1.335929
6	5.067984	5.098328	0.961679
1	5.297104	6.004975	0.402064
1	5.915360	4.472761	1.234572
1	5.685358	2.549044	0.592169
6	2.692046	5.780311	1.024210
1	2.306561	6.256003	1.938101
1	3.029011	6.577570	0.351332
1	1.841217	5.263446	0.556324
6	5.104663	1.863301	1.207018
1	5.569458	0.897055	1.419447
6	2.065752	0.680688	-1.541085
7	2.168017	0.722096	-2.886273
7	0.914464	0.022175	-1.291493
6	1.087890	0.088690	-3.480333
1	0.993691	0.017411	-4.556226
6	0.294077	-0.350862	-2.472125
1	-0.646696	-0.886934	-2.474720
6	0.417114	-0.219365	0.033120
6	0.877167	-1.349423	0.723441
6	-0.472487	0.712352	0.585513
6	0.397333	-1.542462	2.020908
6	-0.932612	0.465255	1.880909
6	-0.504009	-0.650652	2.590631
1	0.729550	-2.411334	2.588951
1	-1.629954	1.165124	2.341486
1	-0.872925	-0.824082	3.600396
6	3.286945	1.310433	-3.570366
6	4.416287	0.510910	-3.796504
6	3.214984	2.666122	-3.923857
6	5.519881	1.123671	-4.394126
6	4.345330	3.228544	-4.518712
6	5.485546	2.466631	-4.748683
1	6.420522	0.540558	-4.584801
1	6.357041	2.925950	-5.212878
6	-0.906882	1.961547	-0.153026
1	-0.435054	1.964833	-1.148479
6	1.995043	3.510807	-3.619218
1	1.141308	2.835879	-3.451160
6	1.854365	-2.337099	0.120525
1	2.105207	-2.008065	-0.899935
6	4.473851	-0.947814	-3.390811
1	3.469002	-1.258116	-3.064345
6	3.498096	1.456476	3.132826
1	3.368868	0.410254	2.828345
1	4.199749	1.461866	3.981358
6	3.155203	-2.384620	0.918953
1	2.978823	-2.709376	1.954624
1	3.860294	-3.094693	0.465155
1	3.641573	-1.396113	0.954029
6	1.225664	-3.724078	0.011886
1	0.973431	-4.127291	1.002918
1	0.303716	-3.699689	-0.585448
1	1.922448	-4.426240	-0.465246
6	-2.418446	1.984274	-0.361796
1	-2.760937	1.092757	-0.905159
1	-2.955056	2.021562	0.596692
1	-2.712718	2.869640	-0.941247
6	-0.431017	3.217137	0.576353
1	-0.703476	4.117577	0.007532
1	-0.890267	3.301859	1.572751
1	0.662279	3.214085	0.710344
6	1.619025	4.443329	-4.765895
1	0.666183	4.942866	-4.545594
1	2.369349	5.232273	-4.915109
1	1.506466	3.901015	-5.714016
6	2.211951	4.307077	-2.331174
1	1.312938	4.889413	-2.082508
1	2.440830	3.642440	-1.482417
1	3.052546	5.009390	-2.441609
6	4.868019	-1.845739	-4.560632
1	4.195972	-1.709255	-5.418319
1	5.893531	-1.643446	-4.899731
1	4.825531	-2.901209	-4.259961
6	5.423423	-1.149550	-2.210153
1	5.423668	-2.201905	-1.892894
1	6.455347	-0.881406	-2.480159
1	5.129984	-0.531402	-1.345138
1	4.335450	4.280469	-4.801745

XVIIIc

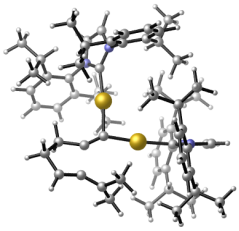


E = -2939.075552 h.
G = -2937.872069 h.

6	2.201757	-0.862918	0.269692
6	2.614109	-0.907941	1.674911
1	3.710380	-0.969054	1.745116
1	2.314439	0.025265	2.175695
6	2.823406	3.007758	-1.531223
7	2.133040	4.120417	-1.194396
7	3.747289	3.423821	-2.424649
6	3.638007	4.786035	-2.649911
1	4.303098	5.304039	-3.329185
6	2.616439	5.225381	-1.874381
1	2.193702	6.211576	-1.727748
6	1.123998	4.168366	-0.172788
6	-0.199152	3.851852	-0.505888
6	-1.148924	3.922937	0.515766
6	0.540183	4.577623	2.107608
6	-0.785015	4.285088	1.806518
1	-2.189607	3.687085	0.294096
1	0.812552	4.849729	3.127282
1	-1.541936	4.337964	2.587767
6	4.768590	2.586937	-2.989912
6	4.531004	1.974771	-4.227912
6	5.963887	2.432991	-2.272116

6	5.571731	1.223642	-4.778096
6	6.966975	1.661250	-2.861396
6	6.778961	1.073802	-4.106327
1	5.433325	0.747056	-5.748595
1	7.912410	1.522295	-2.337167
1	7.578534	0.486472	-4.555192
6	-0.610364	3.410668	-1.893286
1	0.276064	3.437085	-2.546754
1	5.284379	3.599702	-0.608752
6	6.188956	3.045855	-0.904595
6	3.207116	2.096799	-4.953390
1	2.478376	2.566896	-4.272807
6	1.971966	-2.103090	2.399693
1	2.328276	-3.033057	1.930770
1	2.322370	-2.101659	3.439833
6	1.528206	4.523521	1.123197
6	2.974155	4.810093	1.475207
1	3.568469	4.813700	0.549041
6	1.733564	-1.038175	-0.871666
79	2.428554	1.087923	-0.964069
79	0.831633	-1.557052	-2.620733
6	-0.119139	-2.294602	-4.296691
6	-1.652034	-2.831397	-5.865763
1	-2.578358	-2.726548	-6.415707
6	-0.646689	-3.732625	-5.958806
1	-0.506506	-4.590862	-6.603135
7	-1.312053	-1.957981	-4.841595
7	0.283388	-3.388022	-4.991411
6	1.384416	-4.227555	-4.594872
6	2.640771	-4.047157	-5.191181
6	1.134505	-5.195603	-3.609670
6	3.673048	-4.886423	-4.767299
6	2.203825	-6.001915	-3.215363
6	3.459333	-5.850286	-3.788573
1	4.662883	-4.784879	-5.209370
1	2.045044	-6.760496	-2.448868
1	4.281847	-6.490164	-3.472458
6	-2.203328	-0.925978	-4.380501
6	-2.305430	0.252714	-5.132548
6	-2.992262	-1.179627	-3.244423
6	-3.287236	1.173531	-4.755958
6	-3.950168	-0.222020	-2.907216
6	-4.109231	0.933348	-3.663447
1	-3.409296	2.092057	-5.329529
1	-4.590308	-0.390132	-2.042170
1	-4.873312	1.659366	-3.388874
6	-1.396723	0.547424	-6.306969
1	-0.596030	-0.209378	-6.321779
6	-2.862312	-2.450951	-2.430354
1	-1.876169	-2.890568	-2.636240
6	-0.229958	-5.395076	-2.983121
1	-0.927292	-4.667355	-3.423176
6	2.867011	-3.027932	-6.287184
1	2.113613	-2.231143	-6.174123
6	0.468224	-2.056520	2.362064
1	-0.001136	-2.218823	1.383824
6	-0.288678	-1.809924	3.402710
6	-1.043217	-1.570412	4.449148
6	-1.441709	-0.175153	4.842371
1	-2.537405	-0.073741	4.842047
1	-1.105166	0.049521	5.865573
1	-1.025229	0.581030	4.166750
6	-1.571180	-2.674278	5.322247
1	-1.245886	-3.663765	4.981597
1	-1.236787	-2.538606	6.361658
1	-2.671333	-2.658153	5.340335
6	3.543255	3.709303	2.369547
1	4.598230	3.913559	2.600621
1	2.998426	3.648438	3.322931
1	3.485712	2.722691	1.883995
6	3.136127	6.182044	2.123852
1	2.740902	6.980079	1.480281
1	2.614020	6.238482	3.089164
1	4.197653	6.392421	2.312117
6	-1.656917	4.342302	-2.497037
1	-2.589357	4.328919	-1.914358
1	-1.298875	5.380253	-2.536638
1	-1.902067	4.027857	-3.521201
6	-1.116948	1.970321	-1.858166
1	-2.050720	1.894798	-1.281368
1	-1.320851	1.604185	-2.875911
1	-0.379436	1.299012	-1.392262
6	7.346527	4.041097	-0.930549
1	8.294164	3.544728	-1.183465
1	7.176931	4.836858	-1.669367
1	7.470688	4.512613	0.054016
6	6.421368	1.960902	0.145366
1	7.330617	1.382360	-0.071602
1	6.544842	2.409213	1.140907
1	5.578593	1.253681	0.188435
6	3.335512	2.988973	-6.185736
1	3.698769	3.992238	-5.923468
1	4.038928	2.558581	-6.913468
1	2.362858	3.101123	-6.685446
6	2.657912	0.722203	-5.328420
1	1.651291	0.814903	-5.759459
1	3.290873	0.225760	-6.077333
1	2.589641	0.060302	-4.449844
6	4.242859	-2.375969	-6.213950
1	5.047434	-3.089065	-6.441202
1	4.315594	-1.569604	-6.956863
1	4.437768	-1.947961	-5.220495
6	2.664156	-3.680759	-7.655042
1	3.398717	-4.485464	-7.807477
1	1.662369	-4.120032	-7.756804
1	2.796288	-2.945205	-8.460476
6	-0.203303	-5.145832	-1.476296
1	-1.218514	-5.223514	-1.059953
1	0.425827	-5.884990	-0.959283
1	0.187722	-4.144202	-1.236064
6	-0.774957	-6.786592	-3.296930
1	-0.826274	-6.962948	-4.380425
1	-0.142538	-7.572142	-2.859171
1	-1.786862	-6.905019	-2.884840
6	-2.152223	0.454485	-7.630935
1	-2.606658	-0.535472	-7.772635
1	-2.957833	1.201393	-7.677823
1	-1.474807	0.641038	-8.475337
6	-0.732317	1.915242	-6.163036
1	0.004548	2.066320	-6.964692
1	-1.463811	2.732190	-6.238511
1	-0.211906	2.011518	-5.197220
6	-3.918781	-3.470214	-2.851544
1	-4.931670	-3.084943	-2.661670
1	-3.846556	-3.709567	-3.922125
1	-3.802363	-4.405920	-2.285558
6	-2.915428	-2.195750	-0.927313
1	-3.913115	-1.879741	-0.591550
1	-2.669695	-3.118164	-0.382152
1	-2.194619	-1.422294	-0.622853

$TS_{XVIIIe\text{-}XIXe}$



E = -2939.049742 h.
G = -2937.840000 h.

The energy of **$TS_{XVIIIe\text{-}XIXe}$** was calculated by freezing the following distances: *d*(C1-C79) and *d*(C1-C80). The values of these distances were taken from the optimized geometry using a simplified ligand (Me instead of *i*Pr) and B3LYP as functional.

6	1.232185	-0.475116	1.313865
6	1.486940	0.429330	2.488856
1	2.117060	1.264164	2.156077
1	0.520557	0.857389	2.798197
6	2.662966	2.949929	-1.822206
7	2.202729	4.180825	-1.477977
7	3.605119	3.181586	-2.767820
6	3.724179	4.543384	-3.021136
1	4.433698	4.924605	-3.744602
6	2.838680	5.170274	-2.212665
1	2.608877	6.218794	-2.069620
6	1.414817	4.445399	-0.299826
6	0.018188	4.345956	-0.345640
6	-0.685995	4.634305	0.826484
6	1.362281	5.053293	2.017241
6	-0.024858	4.989103	1.994602
1	-1.774200	4.576989	0.819397
1	1.877436	5.311638	2.942512
1	-0.594644	5.211995	2.895568
6	4.523589	2.212759	-3.309008
6	4.368226	1.796315	-4.638081
6	5.593008	1.784666	-2.500950
6	5.354311	0.965771	-5.176268
6	6.539464	0.939717	-3.083735
6	6.433560	0.545637	-4.411520
1	5.268349	0.640725	-6.213203
1	7.384462	0.597066	-2.487325
1	7.191865	-0.102359	-4.848780
6	-0.740453	3.922905	-1.583264
1	-0.011742	3.674467	-2.370022
1	4.853771	2.722075	-0.728315
6	5.772504	2.220268	-1.061389
6	3.172936	2.173506	-5.484584
1	2.485221	2.775618	-4.870147
6	2.087570	-0.337777	3.653744
1	3.184819	-0.403525	3.570434
1	1.874026	0.151053	4.612995
6	2.113612	4.779936	0.873378
6	3.626537	4.808494	0.958771
1	4.045166	4.614495	-0.039190
6	1.092816	-0.432773	0.040258
79	1.922617	1.213056	-0.995297
79	0.261555	-1.337835	-1.619994
6	-0.461053	-2.147546	-3.393671
6	-1.518753	-2.506025	-5.361802
1	-2.263440	-2.325278	-6.127099
6	-0.510967	-3.404564	-5.276512
1	-0.184539	-4.189270	-5.947143
7	-1.477283	-1.748494	-4.198065
7	0.117817	-3.178828	-4.061538
6	1.072446	-4.084286	-3.478835
6	2.437244	-3.770821	-3.506161
6	0.571185	-5.260083	-2.893676
6	3.318938	-4.683490	-2.921667
6	1.495011	-6.142132	-2.330482
6	2.855440	-5.857465	-2.342274
1	4.387496	-4.467550	-2.925461
1	1.140791	-7.067632	-1.876091
1	3.560654	-6.559027	-1.899046
6	-2.482519	-0.772250	-3.873169
6	-2.431112	0.482742	-4.492930
6	-3.525071	-1.153052	-3.007910
6	-3.485196	1.367707	-4.248701
6	-4.540933	-0.223385	-2.782972
6	-4.530160	1.019625	-3.405470
1	-3.478789	2.349034	-4.723903
1	-5.368142	-0.486095	-2.125414
1	-5.341815	1.723208	-3.227087
6	-1.286303	0.913862	-5.383742
1	-0.569024	0.082523	-5.460596
6	-3.615855	-2.539270	-2.401664
1	-2.604317	-2.970109	-2.359695
6	-0.907223	-5.594262	-2.857445
1	-1.468750	-4.754813	-3.293355
6	2.971469	-2.492975	-4.110177
1	2.119935	-1.906899	-4.488448
6	1.484438	-1.701818	3.570798
1	1.519563	-2.389347	4.416292
6	0.923687	-2.053010	2.424829
6	0.313220	-3.028476	1.693315
6	1.131154	-3.821804	0.761568
1	2.159985	-3.977887	1.104386
1	0.661729	-4.774476	0.483864
1	1.182763	-3.209157	-0.178262
6	-1.136293	-2.964498	1.412454
1	-1.697397	-2.378202	2.148522
1	-1.235323	-2.461780	0.419904
1	-1.579604	-3.963196	1.301671
6	-1.572213	2.670788	-1.306704
1	-2.355147	2.863142	-0.558823
1	-2.073303	2.333137	-2.224921
1	-0.945853	1.842625	-0.937301
6	-1.618638	5.057671	-2.104686
1	-2.367667	5.357092	-1.357616
1	-1.021359	5.945110	-2.356670
1	-2.160990	4.744924	-3.008714
6	4.128801	3.701350	1.884048
1	5.224480	3.736077	1.967673
1	3.715713	3.810587	2.897621
1	3.843865	2.706078	1.509083
6	4.148162	6.172554	1.402400
1	3.790413	6.975718	0.743307
1	3.836493	6.415402	2.428310
1	5.246956	6.181044	1.380723
6	6.912330	3.229584	-0.937698
1	7.874035	2.786766	-1.235604
1	6.738242	4.111379	-1.570962
1	7.011671	3.574905	0.101527
6	5.980393	1.028128	-0.130956
1	6.920703	0.498620	-0.339928
1	6.022505	1.365389	0.914179
1	5.156943	0.302910	-0.219960
6	3.578313	3.010542	-6.694511
1	4.114405	3.922692	-6.399009
1	4.234401	2.440648	-7.368383
1	2.690392	3.309962	-7.268854
6	2.422067	0.916977	-5.923524

1	1.543944	1.180551	-6.529039
1	3.056377	0.264102	-6.540326
1	2.076765	0.335470	-5.054274
6	3.683181	-1.647341	-3.054507
1	3.888102	-0.641618	-3.449926
1	3.070370	-1.538773	-2.145753
1	4.644865	-2.095859	-2.762052
6	3.894509	-2.780037	-5.291115
1	4.763842	-3.378437	-4.982447
1	3.373991	-3.327478	-6.089264
1	4.277863	-1.841062	-5.715583
6	-1.207300	-6.835289	-3.694710
1	-2.287556	-7.036502	-3.710467
1	-0.867735	-6.716415	-4.732874
1	-0.707674	-7.722794	-3.280086
6	-1.413078	-5.765929	-1.427943
1	-2.492458	-5.974471	-1.427430
1	-0.918659	-6.604669	-0.916523
1	-1.237451	-4.856973	-0.835038
6	-1.768079	1.241164	-6.794515
1	-2.449335	2.103956	-6.797391
1	-0.916611	1.491540	-7.442482
1	-2.299392	0.392379	-7.246997
6	-0.549802	2.099959	-4.762512
1	-0.077172	1.813728	-3.809759
1	0.234744	2.466587	-5.439213
1	-1.232864	2.939062	-4.566433
6	-4.465420	-3.444316	-3.294878
1	-5.492914	-3.058704	-3.371938
1	-4.056565	-3.513318	-4.312783
1	-4.518761	-4.462159	-2.881852
6	-4.156203	-2.529507	-0.975392
1	-5.220866	-2.258720	-0.937671
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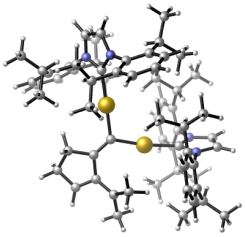
XIXc



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G = -2937.850435 h.

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1	1.448073	1.445955	2.038171
6	2.774818	3.098944	-1.901915
7	2.442596	4.360150	-1.516431
7	3.738416	3.278278	-2.841223
6	3.999150	4.630094	-3.040216
1	4.747201	4.966173	-3.747039
6	3.181064	5.310659	-2.206124
1	3.063636	6.370549	-2.016467
6	1.673966	4.654134	-0.335474
6	0.278438	4.759551	-0.418222
6	-0.411378	5.064064	0.756963
6	1.641547	5.102618	2.016175
6	0.261133	5.237108	1.961209
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1	2.158303	5.224476	2.968109
1	-0.298907	5.475085	2.864559
6	4.541413	2.252190	-3.452384
6	4.332782	1.947889	-4.805816
6	5.566091	1.659701	-2.693237
6	5.222902	1.059945	-5.415541
6	6.419951	0.770542	-3.349231
6	6.262086	0.482817	-4.698833
1	5.098767	0.816826	-6.470857
1	7.231003	0.303118	-2.791353
1	6.948293	-0.204025	-5.192462
6	-0.456798	4.589052	-1.730007
1	0.167299	3.965760	-2.390269
1	4.919326	2.511501	-0.844804
6	5.792305	1.964841	-1.226638
6	3.187124	2.534111	-5.602052
1	2.527629	3.073523	-4.904063
6	0.693416	-0.036571	3.495287
1	1.205460	-0.026398	4.466475
1	-0.192223	0.614416	3.622424
6	2.379946	4.807308	0.868173
6	3.880221	4.622189	0.974428
1	4.293064	4.463634	-0.032844
6	1.064139	-0.276369	-0.166122
79	1.922386	1.385539	-1.038609
79	0.162489	-1.415688	-1.630666
6	-0.613657	-2.400478	-3.312521
6	-1.742408	-2.798596	-5.237225
1	-2.529453	-2.652530	-5.966623
6	-0.700894	-3.663313	-5.193553
1	-0.378421	-4.442076	-5.873758
7	-1.669821	-2.038407	-4.079328
7	-0.029743	-3.411415	-4.006365
6	1.062658	-4.199714	-3.509913
6	2.369237	-3.700297	-3.609324
6	0.760973	-5.440754	-2.923453
6	3.398487	-4.489221	-3.089938
6	1.826699	-6.187110	-2.415966
6	3.131743	-5.716803	-2.496391
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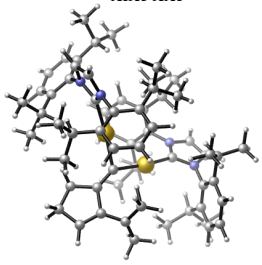

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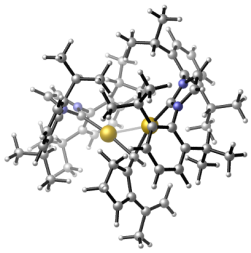

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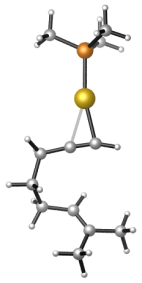
1	1.361879	1.899427	-6.709198
1	2.760686	0.876188	-7.058689
1	1.894132	0.685966	-5.514084
6	-0.628189	2.005196	-4.241457
1	0.112709	2.334457	-4.981731
1	-1.183662	2.895359	-3.917304
1	-0.087479	1.605815	-3.365587
6	-2.291385	1.507125	-6.065671
1	-2.962433	0.758235	-6.508748
1	-2.896154	2.389599	-5.811570
1	-1.567272	1.811003	-6.834493
6	-4.574999	-3.464870	-2.366375
1	-5.532107	-3.041766	-2.026969
1	-4.562811	-3.429804	-3.464677
1	-4.545277	-4.521209	-2.062286
6	-3.399063	-2.798478	-0.244186
1	-4.320924	-2.393510	0.196455
1	-3.334125	-3.851385	0.062452
1	-2.544723	-2.266525	0.201490
6	3.336377	-1.727124	-4.146641
1	3.520927	-0.713912	-4.532046
1	2.838254	-1.632261	-3.168690
1	4.312355	-2.208829	-3.983898
6	3.206386	-2.669475	-6.472329
1	4.192102	-3.143513	-6.359188
1	2.623961	-3.268088	-7.185741
1	3.369610	-1.677885	-6.917750
6	-0.906108	-5.907097	-1.466808
1	-1.932716	-6.102661	-1.125722
1	-0.286535	-6.756574	-1.145354
1	-0.538943	-5.009219	-0.948392
6	-1.435933	-6.961750	-3.692902
1	-1.434724	-6.830729	-4.783888
1	-0.847462	-7.861114	-3.462225
1	-2.470764	-7.149815	-3.374799

6.3 Coordinates and Energies of Relevant Intermediates and Transition States (B3LYP, L_1 = PMe_3, a series; L_2 = 1,3-bis(2,6-dimethylphenyl)imidazol-2-ylidene), b series).

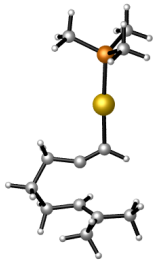
Ia



E = -948.116792 h.
G = -948.116792 h.

6	0.790236	0.073922	0.734295
1	-0.283372	0.037078	0.757657
6	1.977956	-0.047761	1.038417
6	3.358788	-0.276194	1.477145
1	3.910683	-0.720948	0.640777
1	3.833571	0.688463	1.696437
6	3.102829	-0.584698	4.067168
1	3.387917	-1.303952	4.842794
1	3.741573	0.297292	4.218335
6	1.658919	-0.174694	4.225876
1	1.398697	0.789713	3.787750
6	0.673680	-0.852208	4.841995
6	0.837243	-2.196896	5.507459
1	0.530737	-2.146868	6.561851
1	0.183618	-2.942778	5.033139
1	1.860308	-2.580033	5.471453
6	-0.725272	-0.286539	4.914267
1	-1.453523	-0.971170	4.456111
1	-1.044318	-0.153775	5.958073
1	-0.803991	0.682431	4.409515
79	1.643990	1.094906	-1.063948
15	1.994560	2.208338	-3.074843
6	3.705880	2.032254	-3.705942
1	3.932928	0.973637	-3.864652
1	3.811397	2.571539	-4.653852
1	4.413152	2.440055	-2.977098
6	1.688403	4.010941	-2.965969
1	1.847060	4.480462	-3.943027
1	0.658604	4.191714	-2.642674
1	2.369823	4.456389	-2.234668
6	0.908380	1.601395	-4.419548
1	-0.140778	1.733458	-4.137274
1	1.107574	2.159200	-5.341405
1	1.095623	0.537174	-4.592923
6	3.470872	-1.215189	2.707003
1	2.869355	-2.114742	2.532393
1	4.519465	-1.533008	2.746844

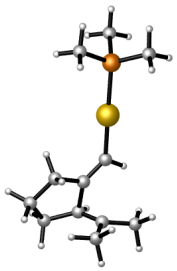
TS_{Ia-IIa}



E = -948.104947 h.
G = -947.834457 h.

6	1.195085	0.886457	1.476530
1	0.218207	1.133750	1.880433
6	2.160147	0.322662	2.118982
6	3.567017	-0.159317	2.044736
1	3.735161	-0.531654	1.027574
1	4.235232	0.698002	2.203846
6	3.363445	-0.705175	4.447064
1	3.286723	-1.518925	5.177172
1	4.083819	0.017821	4.843584
6	2.032226	-0.005034	4.266070
1	2.001851	1.060194	4.487741
6	0.815542	-0.644199	4.168514
6	0.652843	-2.130940	4.067419
1	-0.101851	-2.466565	4.789944
1	0.268694	-2.401406	3.074570
1	1.576928	-2.683816	4.243303
6	-0.451240	0.150219	4.175063
1	-1.085981	-0.110341	3.317249
1	-1.030180	-0.108394	5.073050
1	-0.271858	1.228178	4.185091
79	1.489155	1.403595	-0.538705
15	1.689932	2.000661	-2.796559
6	3.310475	1.574278	-3.546183
1	3.478110	0.494709	-3.477295
1	3.332925	1.875539	-4.599483
1	4.113213	2.087761	-3.007355
6	1.488571	3.797671	-3.116245
1	1.586691	4.006017	-4.187493
1	0.502515	4.127292	-2.773465
1	2.253585	4.357693	-2.569066
6	0.448425	1.188471	-3.877351
1	-0.560500	1.457472	-3.548803
1	0.583647	1.502349	-4.918412
1	0.557885	0.101349	-3.811794
6	3.859408	-1.238104	3.090531
1	3.329393	-2.158680	2.823668
1	4.929332	-1.466684	3.115009

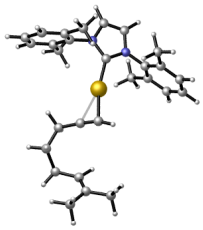
IIa



E = -948.120946 h.
G = -947.847878 h.

6	1.186819	1.087330	1.658401
1	0.351024	1.576812	2.159558
6	1.952416	0.276834	2.443243
6	3.168422	-0.523093	1.993699
1	2.871204	-1.436247	1.465734
1	3.712486	0.091753	1.269801
6	3.319935	-0.201305	4.471801
1	3.247138	-0.899167	5.312492
1	3.871394	0.674616	4.825467
6	1.930694	0.272750	4.042017
1	1.599538	1.221066	4.460176
6	0.864275	-0.634424	3.703251
6	1.031142	-2.118297	3.545520
1	0.609710	-2.578838	4.450894
1	0.449106	-2.493378	2.697697
1	2.062834	-2.453876	3.457034
6	-0.561939	-0.172995	3.834128
1	-1.204288	-0.572143	3.043787
1	-0.928313	-0.574711	4.790014
1	-0.658691	0.913072	3.881599
79	1.432359	1.480098	-0.337053
15	1.682364	1.968854	-2.643501
6	3.088105	1.100683	-3.447632
1	2.951680	0.018112	-3.358691
1	3.151718	1.369219	-4.507947
1	4.024058	1.374823	-2.950129
6	1.970663	3.747653	-3.001207
1	2.082607	3.911333	-4.078789
1	1.125754	4.338054	-2.632494
1	2.878528	4.083721	-2.489787
6	0.220815	1.523387	-3.664349
1	-0.657413	2.073510	-3.311323
1	0.399168	1.766886	-4.717627
1	0.019193	0.451295	-3.572343
6	4.028658	-0.836907	3.243706
1	4.144391	-1.916508	3.375978
1	5.037018	-0.427064	3.135805

Ib

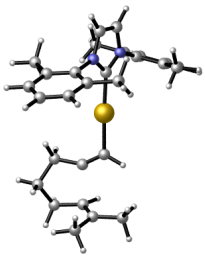


E = -1332.591887 h.
G = -1332.112133 h.

6	2.608789	0.297987	1.513928
1	3.601772	-0.074567	1.686122
6	1.390901	0.480642	1.583181
6	-0.050962	0.625931	1.820131
1	-0.278249	1.696992	1.873428
1	-0.601741	0.226035	0.959361
6	-0.674074	-1.592999	3.068280
1	-1.160915	-1.907638	3.997736
1	-1.373996	-1.839508	2.256872
6	0.608192	-2.359518	2.853749
1	0.959462	-2.396981	1.821809
6	1.350828	-2.998652	3.775257
6	1.032390	-3.060347	5.249484
1	0.956299	-4.103873	5.586260
1	1.843229	-2.607374	5.837616
1	0.103098	-2.551018	5.517616
6	2.609887	-3.733597	3.378912
1	3.486585	-3.333846	3.908737
1	2.546917	-4.797389	3.649707
1	2.802906	-3.669105	2.302516
79	2.386594	1.750800	-0.140040
6	2.690465	3.044043	-1.681100
7	2.238819	4.320641	-1.788795
7	3.424421	2.824661	-2.802632
6	3.433775	3.957752	-3.607524
1	3.967346	3.984905	-4.544965
6	2.686999	4.896907	-2.971630
1	2.432923	5.910119	-3.242072
6	1.410910	4.995806	-0.813183
6	0.015513	4.981544	-0.990651
6	-0.763987	5.649401	-0.037362
6	1.215280	6.313739	1.182784
6	-0.171821	6.306551	1.040897
1	-1.844498	5.654338	-0.152075
1	1.675037	6.836799	2.016928
1	-0.793124	6.822543	1.767940
6	4.116512	1.593401	-3.116358
6	3.441181	0.615326	-3.868147
6	5.444112	1.440033	-2.678213
6	4.135394	-0.565329	-4.162542
6	6.095917	0.242300	-2.999430
6	5.447961	-0.752890	-3.730403
1	3.637394	-1.337996	-4.741588
1	7.122935	0.098632	-2.674903
1	5.971266	-1.674068	-3.972096
6	-0.636987	4.278461	-2.156485
1	-0.245686	4.630860	-3.117822
1	-0.472148	3.194576	-2.120259
1	-1.716766	4.452568	-2.148995
1	5.732418	2.603571	-0.873733
6	6.152417	2.509783	-1.883237
1	7.214381	2.268474	-1.780562
1	6.072128	3.494069	-2.358193
6	2.022082	0.810401	-4.344877
1	1.904043	1.745069	-4.905227
1	1.723578	-0.014758	-4.997980
1	1.314733	0.845660	-3.506841
6	-0.533191	-0.056629	3.126500
1	0.129115	0.230909	3.951385
1	-1.519158	0.371012	3.343983
6	2.038147	5.660017	0.256209
6	3.538310	5.672635	0.420371
1	3.916803	4.684343	0.710561

1	4.049931	5.956594	-0.506113
1	3.829999	6.381841	1.200375

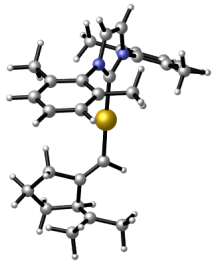
$TS_{Ib\text{-}IIb}$



E = -1332.578163 h.
G = -1332.093412 h.

6	0.860312	0.133448	0.980492
1	-0.034847	-0.354428	0.606568
6	1.414961	-0.092429	2.122702
6	2.517769	0.284387	3.050200
1	3.401527	0.505803	2.440955
1	2.229016	1.206719	3.572443
6	1.462404	-1.233367	4.691990
1	1.563763	-2.178337	5.237757
1	1.138270	-0.476696	5.414020
6	0.415053	-1.338369	3.602984
1	-0.440257	-0.668903	3.672762
6	0.293792	-2.398725	2.732212
6	1.267278	-3.536148	2.647607
1	0.717453	-4.485756	2.648890
1	1.811158	-3.496332	1.694315
1	1.994785	-3.551234	3.461036
6	-0.877995	-2.480488	1.805860
1	-0.551818	-2.638332	0.769035
1	-1.483791	-3.358088	2.072787
1	-1.519129	-1.596977	1.858718
79	1.715605	1.574594	-0.270339
6	2.493313	2.963199	-1.570560
7	1.966396	4.173037	-1.902450
7	3.641217	2.870292	-2.295400
6	3.829014	4.009578	-3.071617
1	4.685355	4.124018	-3.718016
6	2.776120	4.828611	-2.824362
1	2.525157	5.804004	-3.211603
6	0.734095	4.717659	-1.377273
6	-0.470886	4.412008	-2.035012
6	-1.649831	4.962211	-1.514868
6	-0.409434	6.083780	0.231768
6	-1.621434	5.787770	-0.391450
1	-2.594337	4.742954	-2.005607
1	-0.389224	6.735582	1.101089
1	-2.545878	6.208072	-0.004604
6	4.550976	1.746598	-2.277837
6	4.363313	0.713001	-3.213467
6	5.611045	1.753609	-1.353476
6	5.268779	-0.355676	-3.187618
6	6.489608	0.662349	-1.366116
6	6.320795	-0.383658	-2.272720
1	5.146744	-1.165768	-3.901566
1	7.316543	0.644453	-0.661042
1	7.016020	-1.218958	-2.272241
6	-0.512378	3.515753	-3.248802
1	0.210816	3.826065	-4.011605
1	-0.278985	2.476120	-2.986304
1	-1.508638	3.530675	-3.700245
1	4.994664	2.917375	0.367788
6	5.806048	2.882400	-0.369910
1	6.746831	2.755351	0.173512
1	5.832004	3.858553	-0.867756
6	3.229224	0.731383	-4.209224
1	3.194309	1.670030	-4.773887
1	3.336497	-0.089516	-4.924453
1	2.257247	0.616752	-3.713714
6	2.808808	-0.814508	4.075207
1	3.281908	-1.664846	3.572978
1	3.504675	-0.450708	4.837496
6	0.796165	5.559093	-0.251719
6	2.103563	5.888408	0.427419
1	2.548023	5.001687	0.896067
1	2.843404	6.284712	-0.277575
1	1.949826	6.636744	1.210392

IIb

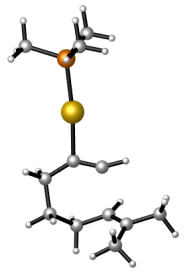


E = -1332.595915 h.
G = -1332.109042 h.

6	0.716052	0.293592	1.144071
1	-0.356528	0.133149	1.022629
6	1.291987	-0.416315	2.165120
6	2.758776	-0.350673	2.575805
1	3.377365	-1.010116	1.956825
1	3.104921	0.669834	2.386249
6	1.411633	-0.979299	4.594430
1	1.345137	-1.904047	5.177802
1	1.077717	-0.163374	5.242147
6	0.468160	-1.034171	3.395840
1	-0.508296	-0.574326	3.527431
6	0.530722	-2.058651	2.385793
6	1.568177	-3.150317	2.344851
1	1.091838	-4.053252	2.752064
1	1.859614	-3.376611	1.314184
1	2.460060	-2.954865	2.937234
6	-0.704773	-2.363389	1.571863
1	-0.464097	-2.614038	0.534255
1	-1.172070	-3.248370	2.025330
1	-1.443970	-1.560537	1.593363
79	1.597307	1.587543	-0.151913
6	2.430753	2.939064	-1.486380
7	1.928189	4.151116	-1.848917
7	3.589702	2.819701	-2.189978
6	3.806864	3.941864	-2.982567
1	4.674414	4.032563	-3.617735
6	2.762148	4.780585	-2.766494
1	2.532297	5.753116	-3.173655
6	0.694983	4.719290	-1.351636
6	-0.503185	4.421810	-2.025617
6	-1.683741	4.988583	-1.527439
6	-0.457261	6.111948	0.227958
6	-1.663102	5.823010	-0.410419
1	-2.623113	4.775855	-2.030831

1	-0.442725	6.771960	1.091199
1	-2.588552	6.256501	-0.040922
6	4.482354	1.683252	-2.141983
6	4.292384	0.637514	-3.063621
6	5.531998	1.691207	-1.205894
6	5.186238	-0.440147	-3.013425
6	6.398345	0.590183	-1.193028
6	6.228234	-0.466410	-2.087033
1	5.062762	-1.259180	-3.716847
1	7.216838	0.572945	-0.478185
1	6.914359	-1.308989	-2.067447
6	-0.536992	3.515073	-3.231854
1	0.218532	3.793875	-3.974941
1	-0.345475	2.471080	-2.952679
1	-1.518204	3.557262	-3.713565
1	4.900275	2.899062	0.478961
6	5.728879	2.832185	-0.236960
1	6.652780	2.693115	0.331803
1	5.790364	3.798537	-0.750898
6	3.167636	0.652664	-4.070107
1	3.150330	1.581081	-4.652287
1	3.270390	-0.182606	-4.769129
1	2.189763	0.560341	-3.581502
6	2.854662	-0.717112	4.079246
1	3.486340	-1.597407	4.227467
1	3.315798	0.095107	4.648657
6	0.749624	5.570380	-0.233110
6	2.050504	5.891734	0.462375
1	2.466255	5.010202	0.966136
1	2.812332	6.250562	-0.239093
1	1.898077	6.666350	1.219616

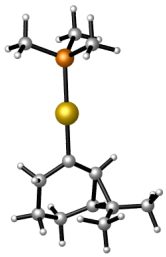
$TS_{Ia\text{-}IIIa}$



E = -948.099130 h.
G = -947.828515 h.

6	1.362718	0.486780	1.930006
1	0.343820	0.822977	1.968419
6	2.479919	0.320183	1.353437
6	3.817786	-0.236522	1.740073
1	4.228101	-0.817486	0.907439
1	4.503583	0.608985	1.889504
6	3.159663	-0.395537	4.244885
1	3.255656	-1.082174	5.096011
1	3.789009	0.471361	4.479008
6	1.717688	0.081981	4.159685
1	1.564702	1.151954	4.294244
6	0.600279	-0.702872	4.194367
6	0.629581	-2.205916	4.177525
1	-0.052564	-2.600396	4.941582
1	0.267563	-2.588854	3.213121
1	1.624072	-2.620288	4.356816
6	-0.769900	-0.086009	4.257973
1	-1.399887	-0.436200	3.427962
1	-1.278504	-0.397259	5.180545
1	-0.736986	1.007810	4.239374
79	2.091223	1.160971	-0.588404
15	1.887065	2.010264	-2.755719
6	3.428150	1.829634	-3.732903
1	3.696303	0.771003	-3.806531
1	3.292807	2.238852	-4.740104
1	4.243500	2.362655	-3.233656
6	1.486868	3.799839	-2.819610
1	1.416954	4.136839	-3.859815
1	0.532449	3.982406	-2.315802
1	2.268548	4.369391	-2.307196
6	0.582645	1.188178	-3.749528
1	-0.389788	1.328677	-3.266854
1	0.549137	1.610182	-4.760096
1	0.790203	0.115380	-3.812683
6	3.741996	-1.104217	3.002285
1	3.161287	-2.006062	2.777804
1	4.758921	-1.433605	3.245767

IIIa

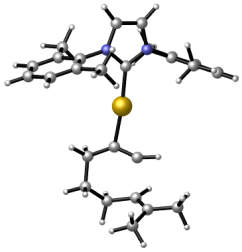


E = -948.128376 h.
G = -947.852596 h.

6	1.337911	0.541952	2.500359
1	0.583800	1.285273	2.267940
6	2.285815	0.228186	1.520570
6	3.516359	-0.564981	1.834714
1	3.488108	-1.467766	1.202509
1	4.345139	0.013883	1.400017
6	3.182088	0.017122	4.311314
1	3.254288	-0.403383	5.322016
1	3.731518	0.966934	4.326519
6	1.729347	0.354260	4.027282
1	1.360417	1.201926	4.603692
6	0.689586	-0.559432	3.577895
6	0.833146	-2.046118	3.309997
1	0.848346	-2.575334	4.271717
1	-0.037991	-2.403589	2.751038
1	1.723962	-2.331683	2.755386
6	-0.742325	-0.170030	3.903329
1	-1.422837	-0.443586	3.090172
1	-1.053279	-0.722673	4.799669
1	-0.846699	0.898843	4.111295
79	2.082525	0.997033	-0.380775
15	1.852529	1.896343	-2.562890
6	3.294317	1.592861	-3.658653
1	3.451630	0.515452	-3.773167
1	3.128712	2.039258	-4.645424
1	4.194210	2.029575	-3.213503
6	1.629353	3.719851	-2.581731
1	1.538236	4.085257	-3.610593
1	0.726235	3.987552	-2.023956
1	2.488420	4.201293	-2.103483
6	0.412604	1.240490	-3.495301
1	-0.509639	1.447172	-2.942932
1	0.351806	1.705466	-4.485490
1	0.511763	0.156560	-3.612698
6	3.831717	-0.938374	3.301131

1	3.525526	-1.965396	3.511124
1	4.917922	-0.917290	3.439841

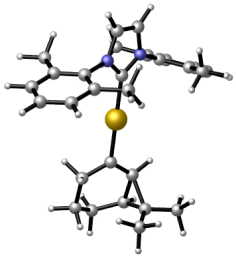
$TS_{Ib\text{-}IIIb}$



E = -1332.572784 h.
G = -1332.088334 h.

6	1.831712	-0.590993	1.407517
1	2.832211	-0.962019	1.289964
6	0.896011	0.232801	1.161434
6	-0.540819	0.366023	1.573921
1	-0.773108	1.421167	1.752462
1	-1.163947	0.057739	0.722690
6	-0.574809	-1.975603	2.686034
1	-0.940138	-2.470502	3.595519
1	-1.171698	-2.376889	1.858575
6	0.873879	-2.378345	2.456817
1	1.070281	-2.939584	1.544417
6	1.883275	-2.337083	3.376250
6	1.746372	-1.737178	4.748569
1	2.187592	-2.410049	5.494946
1	2.303138	-0.792096	4.815295
1	0.709733	-1.542167	5.031234
6	3.233767	-2.915985	3.055119
1	4.028015	-2.168976	3.194659
1	3.461823	-3.739360	3.745646
1	3.289112	-3.303623	2.033167
79	1.854388	1.566349	-0.196003
6	2.601022	2.942967	-1.515176
7	2.323847	4.273584	-1.552763
7	3.458513	2.729846	-2.548911
6	3.714746	3.917397	-3.226995
1	4.373494	3.954395	-4.080850
6	3.001816	4.887530	-2.600499
1	2.910379	5.944696	-2.796450
6	1.444139	4.963944	-0.635808
6	0.079855	5.067365	-0.962130
6	-0.751544	5.743682	-0.059975
6	1.122922	6.191394	1.401366
6	-0.237221	6.297235	1.112201
1	-1.809601	5.838896	-0.288804
1	1.521874	6.634300	2.309916
1	-0.897244	6.821363	1.798170
6	4.026525	1.449211	-2.907801
6	3.301354	0.612448	-3.774830
6	5.292059	1.105896	-2.398191
6	3.874652	-0.619537	-4.115844
6	5.823571	-0.136297	-2.768561
6	5.121654	-0.993241	-3.615956
1	3.335147	-1.283753	-4.785740
1	6.800145	-0.424920	-2.388905
1	5.552039	-1.951240	-3.895088
6	-0.483577	4.474798	-2.230777
1	0.059947	4.818352	-3.118577
1	-0.427370	3.379190	-2.222374
1	-1.534458	4.754362	-2.349385
1	5.540579	2.176189	-0.528823
6	6.061568	2.026749	-1.482552
1	7.047843	1.608048	-1.262541
1	6.208050	3.017474	-1.928088
6	1.950608	1.006992	-4.320730
1	1.964084	2.009582	-4.763177
1	1.629945	0.300272	-5.091554
1	1.186881	1.011871	-3.532857
6	-0.872696	-0.465825	2.817960
1	-0.333964	-0.050479	3.677135
1	-1.942415	-0.349157	3.027854
6	1.994728	5.523991	0.531050
6	3.465664	5.412735	0.851666
1	3.746193	4.379256	1.090868
1	4.092847	5.730904	0.011112
1	3.717401	6.034494	1.715789

IIIb

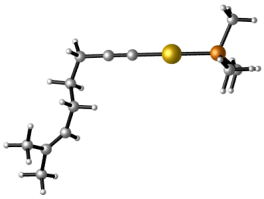


E = -1332.604075 h.
G = -1332.113647 h.

6	1.705904	-1.107243	1.424662
1	2.513681	-1.352637	0.744481
6	1.056629	0.126330	1.257649
6	-0.236376	0.429204	1.952321
1	-0.064742	1.319160	2.580110
1	-0.897775	0.812792	1.161016
6	-0.575479	-2.091341	2.298000
1	-0.936437	-2.829749	3.024919
1	-1.078358	-2.314907	1.348326
6	0.909672	-2.310119	2.072859
1	1.135709	-3.233001	1.539948
6	2.004458	-1.813441	2.898329
6	1.888906	-0.993257	4.170820
1	1.586043	-1.656165	4.991810
1	2.869094	-0.577543	4.427105
1	1.181568	-0.168342	4.125516
6	3.306357	-2.595120	2.838853
1	4.171991	-1.927659	2.908251
1	3.340873	-3.277434	3.698510
1	3.391618	-3.194251	1.927392
79	1.804976	1.494484	-0.064763
6	2.563923	2.876293	-1.409615
7	2.302684	4.210699	-1.466643
7	3.428499	2.646427	-2.435387
6	3.701822	3.822046	-3.125658
1	4.365288	3.843022	-3.976460
6	2.994773	4.806893	-2.514512
1	2.917309	5.862817	-2.723034
6	1.424294	4.920254	-0.563360
6	0.062213	5.029516	-0.896620
6	-0.768559	5.722022	-0.006171
6	1.102570	6.174107	1.457927
6	-0.255628	6.285734	1.161765
1	-1.824916	5.822029	-0.240871
1	1.500837	6.625202	2.362769

1	-0.914946	6.822571	1.838556
6	3.983982	1.355803	-2.777679
6	3.250146	0.513135	-3.631712
6	5.246942	1.007271	-2.264978
6	3.811968	-0.728483	-3.956878
6	5.766762	-0.244666	-2.618740
6	5.056202	-1.106756	-3.453624
1	3.265665	-1.396732	-4.617245
1	6.740975	-0.537025	-2.235865
1	5.477603	-2.072282	-3.720355
6	-0.500091	4.425307	-2.160254
1	0.057997	4.743233	-3.048525
1	-0.463777	3.329116	-2.132433
1	-1.544614	4.721603	-2.293923
1	5.503697	2.100169	-0.410410
6	6.025089	1.932213	-1.360849
1	7.006143	1.505559	-1.132927
1	6.183448	2.915100	-1.819471
6	1.901101	0.910187	-4.180232
1	1.917174	1.911792	-4.624599
1	1.579564	0.202466	-4.949845
1	1.136305	0.917847	-3.393332
6	-0.951794	-0.677286	2.760520
1	-0.742754	-0.570514	3.827179
1	-2.033619	-0.543017	2.653102
6	1.973317	5.490359	0.599330
6	3.442185	5.372803	0.927384
1	3.715422	4.339932	1.177632
1	4.074810	5.678475	0.086254
1	3.694467	6.001586	1.786282

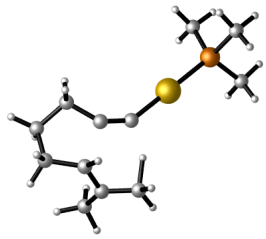
VIIa



E = -947.675851 h.
G = -947.418700 h.

6	-0.043184	1.298969	1.167995
6	1.181510	1.359443	1.230666
6	2.647562	1.425996	1.292832
1	3.006861	0.778481	2.104868
1	2.957995	2.446677	1.561124
79	-2.048754	1.205307	1.059848
15	-4.387657	1.101181	0.919001
6	-5.244818	1.091621	2.545023
1	-6.331601	1.060439	2.408850
1	-4.928506	0.216381	3.121648
1	-4.977846	1.991835	3.107956
6	-5.146407	2.508366	0.012040
1	-4.756631	2.539337	-1.010492
1	-6.236841	2.405596	-0.021124
1	-4.887808	3.448743	0.509238
6	-5.029264	-0.390751	0.059443
1	-6.124732	-0.382417	0.033052
1	-4.644594	-0.418134	-0.965170
1	-4.688551	-1.290862	0.581051
6	3.355359	1.013011	-0.018385
1	4.437375	1.007788	0.166168
1	3.070559	-0.017139	-0.269752
6	3.045116	1.941075	-1.207557
1	1.953285	1.972256	-1.341106
1	3.355901	2.961980	-0.957117
6	5.184172	3.445611	-2.978324
1	4.815702	3.898368	-2.054433
1	6.280024	3.387134	-2.911234
1	4.964173	4.138738	-3.803141
6	5.114623	1.427116	-4.514850
1	6.205138	1.290931	-4.470672
1	4.657102	0.446472	-4.685208
1	4.918442	2.052014	-5.398375
6	3.681316	1.466617	-2.487577
1	3.345153	0.479097	-2.812676
6	4.595100	2.083623	-3.256496

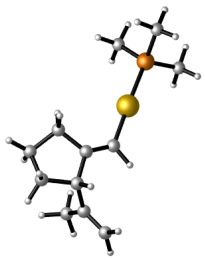
$TS_{VIIa\text{-}VIIIa}$



E = -947.606797 h.
G = -947.349510 h.

6	0.750967	1.973685	-0.702729
6	1.839366	2.275201	-0.104202
6	2.541289	2.392976	1.214793
1	2.036319	1.788036	1.977582
1	2.504606	3.438817	1.556909
79	-1.209885	1.485434	-0.513170
15	-3.477824	0.921122	-0.278844
6	-3.836357	-0.156254	1.167731
1	-4.907358	-0.380049	1.230946
1	-3.278401	-1.093592	1.075014
1	-3.518313	0.345458	2.087368
6	-4.600800	2.359465	-0.049690
1	-4.523340	3.029886	-0.911559
1	-5.639570	2.026741	0.055894
1	-4.308082	2.914376	0.847562
6	-4.203743	0.008870	-1.701803
1	-5.260466	-0.217776	-1.520060
1	-4.116345	0.612951	-2.610676
1	-3.656560	-0.927056	-1.854470
6	4.006368	1.974831	1.030294
1	4.608298	2.191368	1.921087
1	4.050413	0.891539	0.858633
6	4.526348	2.721896	-0.215511
1	4.834428	3.734755	0.072586
1	5.414357	2.225515	-0.623657
6	3.908112	0.612205	-2.422177
1	4.924723	0.619184	-2.013524
1	3.335939	-0.137011	-1.851861
1	3.963741	0.251414	-3.455660
6	2.060679	2.187700	-3.110470
1	1.193862	1.971258	-2.158520
1	1.799334	3.224123	-3.342928
1	1.851284	1.510470	-3.942361
6	3.402952	2.815436	-1.242957
1	3.029079	3.828468	-1.396956
6	3.249852	1.969462	-2.355498

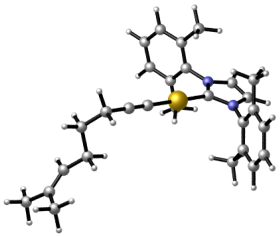
VIIIa



E = -947.684759 h.
G = -947.421768 h.

6	0.630193	2.088013	-1.460452
6	1.730936	2.372391	-0.739248
6	1.875324	2.326569	0.775261
1	1.204474	1.593563	1.236468
1	1.625447	3.309952	1.204994
79	-1.235438	1.539301	-0.796332
15	-3.414239	0.907960	-0.094523
6	-3.469626	-0.384321	1.214830
1	-4.504334	-0.631605	1.478165
1	-2.963217	-1.287965	0.860074
1	-2.947806	-0.025202	2.108032
6	-4.426407	2.279814	0.600081
1	-4.538999	3.069650	-0.149791
1	-5.418641	1.924007	0.900055
1	-3.918847	2.703854	1.472796
6	-4.468920	0.217684	-1.435874
1	-5.461160	-0.051299	-1.056127
1	-4.578566	0.957698	-2.235355
1	-3.991607	-0.674089	-1.855234
6	3.368024	2.039185	1.007470
1	3.712400	2.321586	2.008977
1	3.563932	0.966514	0.881255
6	4.062552	2.843300	-0.108354
1	4.171847	3.888032	0.208104
1	5.067299	2.473749	-0.340543
6	3.875785	0.431969	-2.120279
1	4.676702	0.356706	-1.372820
1	2.997148	-0.069008	-1.695157
1	4.191196	-0.127603	-3.007092
6	3.700476	2.334074	-3.710383
1	0.758787	2.173454	-2.546667
1	3.487435	3.371219	-3.962755
1	4.026790	1.692678	-4.527275
6	3.101249	2.786423	-1.338266
1	3.009460	3.791552	-1.768025
6	3.570225	1.871898	-2.458893

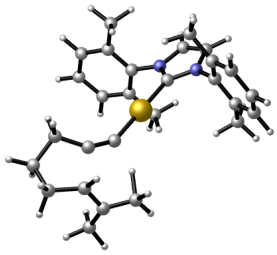
VIIb



E = -1332.147990 h.
G = -1331.679096 h.

6	-1.047607	1.296140	1.091618
6	0.174248	1.371319	1.190954
6	1.636531	1.457241	1.305198
1	1.971558	0.846284	2.155257
1	1.927287	2.490980	1.544809
79	-3.044530	1.183747	0.962282
6	2.401460	1.001853	0.041132
1	3.475083	1.013570	0.269885
1	2.135266	-0.039468	-0.183066
6	2.134998	1.882212	-1.194224
1	1.050794	1.890168	-1.381282
1	2.417914	2.916183	-0.965349
6	4.368308	3.343345	-2.881346
1	3.939166	3.824855	-1.999023
1	5.457117	3.288502	-2.738075
1	4.204965	4.010218	-3.740183
6	4.390091	1.282417	-4.362392
1	5.477049	1.154717	-4.253491
1	3.947942	0.293937	-4.527872
1	4.240773	1.878558	-5.274486
6	2.841438	1.374717	-2.423683
1	2.525905	0.377528	-2.739794
6	3.797546	1.972710	-3.155296
6	-5.095485	1.079517	0.850317
6	-7.292541	1.650999	0.841255
1	-8.136986	2.321099	0.889762
6	-7.223383	0.304127	0.696048
1	-7.995627	-0.442273	0.592101
7	-5.982627	2.111215	0.932457
7	-5.872388	-0.029975	0.703552
6	-5.373648	-1.379987	0.572061
6	-5.208388	-1.913068	-0.719158
6	-5.099337	-2.114580	1.739266
6	-4.736760	-3.227863	-0.822721
6	-4.630034	-3.425556	1.584479
6	-4.446088	-3.976910	0.317216
1	-4.599940	-3.662249	-1.809460
1	-4.411309	-4.014482	2.471201
1	-4.082571	-4.996221	0.217646
6	-5.626889	3.502276	1.097203
6	-5.547203	4.317286	-0.046925
6	-5.405542	3.993327	2.396322
6	-5.215011	5.665376	0.138512
6	-5.074666	5.348059	2.530562
6	-4.977297	6.176925	1.413804
1	-5.144959	6.314275	-0.730379
1	-4.897921	5.750082	3.524601
1	-4.721048	7.225753	1.537716
6	-5.506805	3.105889	3.613069
1	-6.435386	2.523580	3.619269
1	-4.675613	2.391081	3.653658
1	-5.476131	3.706082	4.527418
6	-5.798621	3.774441	-1.433052
1	-5.063144	3.007466	-1.703960
1	-6.790343	3.315179	-1.520302
1	-5.733880	4.576512	-2.174225
6	-5.526191	-1.112092	-1.958662
1	-6.567378	-0.768322	-1.967446
1	-4.893149	-0.220237	-2.037022
1	-5.364513	-1.717085	-2.855580
6	-5.292683	-1.526023	3.115718
1	-4.530593	-0.767781	3.335054
1	-6.269815	-1.040760	3.219986
1	-5.217167	-2.305829	3.879627

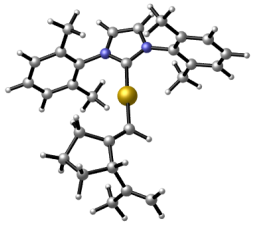
$TS_{VIIb\text{-}VIIIb}$



E = -1332.078201 h.
G = -1331.609153 h.

6	-0.506852	1.650731	0.027772
6	0.656267	1.366687	0.476423
6	1.433380	0.513324	1.433898
1	0.852356	-0.369058	1.728169
1	1.639094	1.085035	2.352269
79	-2.515956	1.431470	0.149163
6	2.764209	0.128869	0.773468
1	3.446556	-0.359907	1.479447
1	2.567950	-0.582026	-0.039842
6	3.360836	1.430114	0.197286
1	3.897293	1.964711	0.991254
1	4.095087	1.207460	-0.585396
6	2.199952	1.378009	-2.693759
1	1.515986	0.515821	-2.638086
1	2.124644	1.778535	-3.711440
1	3.216182	0.989547	-2.561878
6	0.683353	3.225458	-1.886954
1	-0.153513	2.543198	-1.152033
1	0.625914	4.180997	-1.357575
1	0.289256	3.291111	-2.904299
6	2.225238	2.309510	-0.319065
1	2.071020	3.216131	0.268074
6	1.844299	2.428647	-1.668839
6	-4.559743	1.219715	0.280449
6	-6.778039	1.674042	0.466826
1	-7.652198	2.300720	0.553760
6	-6.643419	0.325380	0.419293
1	-7.375645	-0.466635	0.454707
7	-5.494994	2.207221	0.379698
7	-5.281008	0.063296	0.305523
6	-4.719769	-1.265740	0.224851
6	-4.518837	-1.838738	-1.043886
6	-4.422673	-1.944431	1.420608
6	-3.984323	-3.132745	-1.095058
6	-3.891994	-3.236753	1.318466
6	-3.670712	-3.825392	0.073799
1	-3.820240	-3.597100	-2.064019
1	-3.653580	-3.781835	2.227891
1	-3.259605	-4.829694	0.014958
6	-5.206865	3.623111	0.390838
6	-5.230868	4.324812	-0.828182
6	-4.942966	4.249285	1.622392
6	-4.963222	5.699320	-0.791513
6	-4.680582	5.625519	1.608120
6	-4.686923	6.344468	0.413449
1	-4.975275	6.263177	-1.720476
1	-4.474078	6.132433	2.547101
1	-4.482520	7.411831	0.422204
6	-4.931134	3.480484	2.921465
1	-5.838363	2.878955	3.050083
1	-4.077652	2.793052	2.970824
1	-4.856408	4.166501	3.770337
6	-5.525507	3.636875	-2.139449
1	-4.743334	2.912843	-2.397635
1	-6.474676	3.089114	-2.111357
1	-5.582537	4.369424	-2.949864
6	-4.855609	-1.097570	-2.314984
1	-5.874761	-0.694560	-2.296708
1	-4.175695	-0.251951	-2.475697
1	-4.769768	-1.763282	-3.178798
6	-4.651077	-1.314006	2.773315
1	-3.973005	-0.467854	2.939715
1	-5.673171	-0.933390	2.881618
1	-4.475538	-2.043293	3.569841

VIIIb

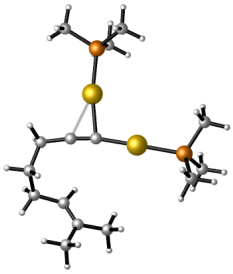


E = -1332.155466 h.
G = -1331.680393 h.

6	-0.536068	2.234946	-0.226994
6	0.559271	1.508368	0.070243
6	0.595740	0.128294	0.713121
1	-0.288664	-0.469570	0.467059
1	0.623647	0.226328	1.810596
79	-2.508927	1.775273	0.083170
6	1.918955	-0.487109	0.227982
1	2.275719	-1.304992	0.864548
1	1.792541	-0.889841	-0.785292
6	2.883836	0.714100	0.209012
1	3.274075	0.883412	1.220533
1	3.749461	0.559673	-0.444615
6	2.083927	1.399324	-2.752945
1	1.080950	0.955095	-2.742310
1	2.242805	1.858248	-3.734446
1	2.799145	0.572469	-2.649424
6	2.562791	3.685339	-1.906634
1	-0.319076	3.204083	-0.695987
1	2.687011	4.420362	-1.113488
1	2.713478	4.039531	-2.924994
6	2.021589	1.946390	-0.210815
1	2.269264	2.796128	0.437417
6	2.243651	2.410502	-1.642231
6	-4.524385	1.337951	0.357760
6	-6.774019	1.549529	0.614762
1	-7.709151	2.078829	0.713652
6	-6.490421	0.223521	0.611233
1	-7.128426	-0.641974	0.702102
7	-5.562199	2.216984	0.459359
7	-5.111327	0.110692	0.454107
6	-4.412123	-1.152539	0.405979
6	-4.152326	-1.734820	-0.847771
6	-4.057523	-1.771248	1.618336
6	-3.500635	-2.974903	-0.865538
6	-3.409001	-3.011034	1.549895
6	-3.131805	-3.608370	0.320591
1	-3.289028	-3.445243	-1.822235
1	-3.123595	-3.508030	2.473290

1	-2.630907	-4.572265	0.287042
6	-5.437595	3.655904	0.419293
6	-5.632160	4.314995	-0.808051
6	-5.157451	4.343501	1.613871
6	-5.523957	5.711649	-0.819918
6	-5.057711	5.739731	1.551876
6	-5.236802	6.418692	0.347396
1	-5.669294	6.243619	-1.756428
1	-4.842258	6.292831	2.462416
1	-5.158192	7.502306	0.319240
6	-4.957091	3.619747	2.922951
1	-5.763526	2.905491	3.125059
1	-4.016490	3.055217	2.924727
1	-4.919656	4.333333	3.751339
6	-5.939578	3.558113	-2.077678
1	-5.126162	2.872449	-2.343126
1	-6.851108	2.955835	-1.983879
1	-6.079506	4.251772	-2.911949
6	-4.540790	-1.053711	-2.137185
1	-5.587694	-0.729056	-2.130721
1	-3.925810	-0.162239	-2.313232
1	-4.399814	-1.730654	-2.985080
6	-4.345540	-1.128836	2.953918
1	-3.788155	-0.191858	3.075252
1	-5.408611	-0.889238	3.073434
1	-4.057659	-1.798046	3.770165

IVa

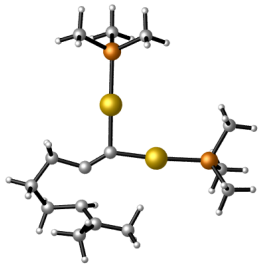


E = -1544.490673 h.
G = -1544.134332 h.

6	3.886965	0.607433	2.517381
1	3.998924	-0.293627	1.901855
1	4.687911	1.293709	2.211651
6	4.429108	1.373094	4.966467
1	4.694612	0.924908	5.930611
1	5.342889	1.857434	4.592661
6	3.364313	2.426992	5.148967
1	3.310832	3.176539	4.358655
6	2.493353	2.548883	6.166945
6	2.407877	1.609033	7.344953
1	2.546063	2.155008	8.289108
1	1.410579	1.149556	7.399652
1	3.144036	0.801972	7.311007
6	1.502438	3.689171	6.205250
1	0.468174	3.315934	6.232515
1	1.635139	4.295791	7.112767
1	1.603735	4.349572	5.337212
79	1.904520	1.640904	-0.082452
15	2.029056	1.765998	-2.394813
6	3.267211	0.630970	-3.131103
1	3.027086	-0.401853	-2.859856
1	3.267145	0.727134	-4.222571
1	4.263024	0.872702	-2.746516
6	2.470905	3.430991	-3.024301
1	2.488336	3.429782	-4.119999
1	1.736735	4.163721	-2.674939

1	3.457372	3.717480	-2.646452
6	0.445836	1.347947	-3.220659
1	-0.336314	2.037539	-2.887980
1	0.553423	1.421019	-4.308546
1	0.149717	0.328072	-2.955692
6	4.079167	0.215670	4.004878
1	3.186230	-0.312192	4.360295
1	4.906361	-0.504448	4.030840
6	2.577175	1.207377	2.217194
6	1.431480	1.680328	2.109775
79	-0.443988	2.453772	2.282134
15	-2.597148	3.343219	2.517939
6	-3.571493	2.579197	3.872137
1	-3.045598	2.711352	4.823071
1	-4.562648	3.041025	3.940626
1	-3.685082	1.506963	3.683216
6	-2.621246	5.143227	2.879189
1	-2.120927	5.687340	2.071655
1	-3.652594	5.501289	2.971264
1	-2.086172	5.338718	3.813935
6	-3.645390	3.154858	1.022426
1	-3.763356	2.092561	0.785932
1	-4.633287	3.599254	1.187430
1	-3.165272	3.650752	0.172683

$TS_{IVa\text{-}Va}$

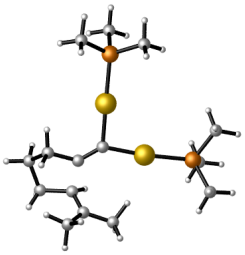


E = -1544.451915 h.
G = -1544.090255 h.

6	4.154472	1.192297	2.826682
1	3.985584	0.259820	2.278779
1	4.694707	1.868407	2.150946
6	4.583059	2.139671	5.028310
1	4.843856	1.943768	6.073823
1	5.120363	3.045144	4.725033
6	3.079062	2.416371	4.869184
1	2.829735	3.473900	4.794420
6	2.125744	1.685840	5.619427
6	2.333374	0.299900	6.132750
1	1.993759	0.243953	7.175066
1	1.697695	-0.403380	5.572578
1	3.364445	-0.047954	6.077216
6	0.791768	2.281813	5.817880
1	0.321662	2.415508	4.806294
1	0.126033	1.668334	6.430344
1	0.853125	3.297305	6.225886
79	1.772261	1.873532	0.343436
15	1.744132	1.565434	-1.990040
6	2.809240	0.186561	-2.572104
1	2.488822	-0.749602	-2.103567
1	2.749622	0.083416	-3.661348
1	3.848523	0.379073	-2.286282
6	2.320686	3.021880	-2.951873
1	2.295915	2.810781	-4.026971
1	1.677829	3.882183	-2.738870

1	3.345067	3.274569	-2.659441
6	0.086371	1.183406	-2.687069
1	-0.601426	2.007151	-2.470360
1	0.144219	1.037855	-3.771743
1	-0.305884	0.272936	-2.222364
6	4.968170	0.978970	4.102355
1	4.714500	0.016268	4.557140
1	6.044292	0.964256	3.899654
6	2.817387	1.859408	3.154172
6	1.773014	2.155250	2.429634
79	-0.115352	2.959371	2.577870
15	-2.284481	3.897925	2.543937
6	-3.439588	3.204211	3.794420
1	-3.032234	3.354264	4.799521
1	-4.418709	3.691234	3.726534
1	-3.561347	2.129062	3.626632
6	-2.307296	5.708226	2.863736
1	-1.714983	6.222920	2.100139
1	-3.333091	6.092663	2.843894
1	-1.864513	5.915677	3.843310
6	-3.186877	3.712125	0.952320
1	-3.286343	2.649651	0.707218
1	-4.184829	4.160048	1.018586
1	-2.624330	4.202664	0.151302

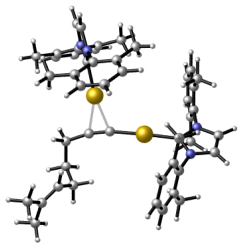
Va



E = -1544.455771 h.
G = -1544.094423 h.

6	3.971116	0.944466	2.981884
1	3.920367	-0.051946	3.443011
1	4.128993	0.802123	1.910079
6	4.447150	2.185099	5.009452
1	4.658347	1.417398	5.759439
1	4.854049	3.127258	5.389790
6	2.920369	2.333099	4.813691
1	2.588233	3.368893	4.763132
6	2.021447	1.504993	5.547128
6	2.323596	0.108836	5.971382
1	2.283480	0.065629	7.070646
1	1.536573	-0.571585	5.618578
1	3.295345	-0.265349	5.648617
6	0.670015	2.022105	5.843056
1	0.171034	2.267363	4.873507
1	0.045441	1.313334	6.393042
1	0.720321	2.977571	6.379760
79	1.747071	1.772097	0.350618
15	1.795159	1.475431	-1.989099
6	2.896243	0.111213	-2.540530
1	2.571948	-0.830205	-2.085283
1	2.873115	0.010264	-3.631389
1	3.923131	0.315273	-2.220052
6	2.385485	2.941557	-2.928669
1	2.393118	2.735468	-4.004969
1	1.728161	3.794503	-2.730542
1	3.398347	3.203779	-2.605956
6	0.168767	1.076578	-2.748830
1	-0.536507	1.891171	-2.554578
1	0.269844	0.937007	-3.831094
1	-0.230337	0.159216	-2.303960
6	5.061274	1.781876	3.656512
1	6.002704	1.236316	3.781056
1	5.266149	2.671946	3.048599
6	2.674891	1.707470	3.214695
6	1.681197	2.055505	2.421964
79	-0.149069	2.980680	2.592537
15	-2.269682	4.033913	2.573364
6	-3.449615	3.385141	3.825351
1	-3.030171	3.508330	4.829194
1	-4.405538	3.917533	3.768073
1	-3.622142	2.318053	3.650571
6	-2.220961	5.843274	2.899127
1	-1.608848	6.337891	2.137901
1	-3.231722	6.265729	2.878633
1	-1.772286	6.031085	3.880049
6	-3.187065	3.892732	0.985287
1	-3.350437	2.836786	0.746238
1	-4.156215	4.399822	1.052783
1	-2.600279	4.345343	0.179400

IVb



E = -2313.441090 h.
G = -2312.655608 h.

6	0.608663	-0.492065	0.317317
6	0.842635	-0.497057	1.774789
1	1.919927	-0.562953	1.970783
1	0.507406	0.457465	2.198253
6	0.510697	-3.073921	2.048506
1	-0.120337	-3.784293	2.593104
1	0.260884	-3.193771	0.984374
6	1.973132	-3.387381	2.245323
1	2.645209	-2.920634	1.522764
6	2.538452	-4.156501	3.192781
6	1.784648	-4.885727	4.278568
1	1.978459	-5.966649	4.226635
1	2.128185	-4.560111	5.270859
1	0.702937	-4.735006	4.235158
6	4.036232	-4.352491	3.236414
1	4.453785	-4.003348	4.191934
1	4.299081	-5.417387	3.157633
1	4.544382	-3.816767	2.427264
6	2.535344	2.866877	-1.493345
7	2.222118	4.149185	-1.164603
7	3.691254	2.955827	-2.204479
6	4.097815	4.280649	-2.317577
1	4.996027	4.557538	-2.847558
6	3.174058	5.030728	-1.663953
1	3.101360	6.095559	-1.505271
6	1.065478	4.552610	-0.395890
6	-0.142918	4.792645	-1.073697
6	-1.248309	5.184492	-0.307222
6	0.071030	5.104894	1.717672
6	-1.145198	5.335250	1.075128

1	-2.193457	5.377245	-0.807855
1	0.151158	5.235579	2.793526
1	-2.012925	5.642281	1.652774
6	4.409035	1.833653	-2.766702
6	4.178576	1.494329	-4.111975
6	5.329643	1.148278	-1.954139
6	4.892860	0.409522	-4.636928
6	6.018604	0.069559	-2.524156
6	5.800695	-0.299929	-3.850857
1	4.734186	0.128022	-5.674564
1	6.736744	-0.475969	-1.917722
1	6.347401	-1.136809	-4.277065
6	-0.266846	4.628033	-2.568652
1	0.537982	5.142187	-3.106460
1	-0.227991	3.570426	-2.858564
1	-1.221332	5.032058	-2.918023
1	4.714007	1.309844	0.116228
6	5.577257	1.544769	-0.518952
1	6.441671	1.007001	-0.118707
1	5.770050	2.619133	-0.419090
6	3.204199	2.259689	-4.974455
1	3.446042	3.328262	-5.015893
1	3.217234	1.873185	-5.997654
1	2.177880	2.176768	-4.597229
6	0.103278	-1.651670	2.490702
1	0.295582	-1.537982	3.564725
1	-0.976109	-1.525845	2.339499
6	1.204855	4.711654	0.994971
6	2.516478	4.465022	1.700724
1	2.803082	3.406951	1.659818
1	3.336780	5.038611	1.254269
1	2.441824	4.748211	2.754680
6	0.272150	-0.715197	-0.862713
79	1.508849	1.182621	-0.994236
79	-0.438121	-1.376940	-2.634617
6	-1.207114	-2.110982	-4.388506
6	-2.410419	-2.339189	-6.295526
1	-3.102694	-2.039296	-7.066779
6	-1.696126	-3.480296	-6.126498
1	-1.637951	-4.379263	-6.720163
7	-2.101038	-1.510645	-5.221916
7	-0.963550	-3.324848	-4.954356
6	-0.076784	-4.333099	-4.416605
6	1.276620	-4.316459	-4.798365
6	-0.613273	-5.309590	-3.557415
6	2.109722	-5.314945	-4.276396
6	0.259562	-6.286219	-3.061262
6	1.608856	-6.288744	-3.413525
1	3.158902	-5.325030	-4.559545
1	-0.130946	-7.051793	-2.396262
1	2.269750	-7.057238	-3.021627
6	-2.668500	-0.195529	-5.025006
6	-2.046451	0.904393	-5.642842
6	-3.834456	-0.073534	-4.248406
6	-2.620578	2.167321	-5.448324
6	-4.371311	1.210081	-4.082698
6	-3.770235	2.320780	-4.673565
1	-2.160109	3.032880	-5.917120
1	-5.274284	1.330884	-3.490087
1	-4.204587	3.307685	-4.538015
6	-0.806352	0.745176	-6.488552
1	0.029803	0.340889	-5.906046
1	-0.971856	0.061745	-7.330056
1	-0.495981	1.711345	-6.897008
6	-4.496360	-1.270097	-3.609005
1	-4.652040	-2.083312	-4.327077
1	-3.888254	-1.674198	-2.790137
1	-5.469893	-0.991925	-3.195004
6	-2.071118	-5.317496	-3.166157
1	-2.321411	-4.455724	-2.535145
1	-2.731824	-5.281282	-4.039921
1	-2.308199	-6.223549	-2.600773
6	1.836508	-3.265248	-5.726028
1	1.203618	-3.113669	-6.607374
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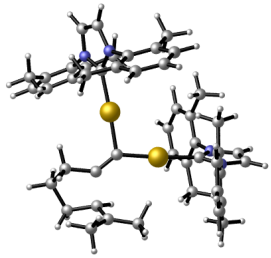

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1	1.635992	0.565510	1.937280
6	-0.833447	-1.534587	3.014529
1	-0.487872	-2.209114	3.803550
1	-1.911416	-1.405257	3.153678
6	-0.574729	-2.161459	1.631509
1	-1.416345	-2.100826	0.944596
6	0.181129	-3.349289	1.495972
6	1.239889	-3.788252	2.452823
1	0.978420	-4.788482	2.828610
1	2.197132	-3.906746	1.926637
1	1.382145	-3.126089	3.306782
6	-0.041327	-4.201896	0.303312
1	0.046830	-3.571537	-0.608116
1	0.662485	-5.035697	0.231972
1	-1.069381	-4.587248	0.290814
6	2.614849	2.706306	-1.583318
7	2.244787	3.972092	-1.235874
7	3.773895	2.869728	-2.282031
6	4.119904	4.215911	-2.367832
1	5.009721	4.544983	-2.881845
6	3.157544	4.908770	-1.710773
1	3.032948	5.966043	-1.534304
6	1.069115	4.318040	-0.470166
6	-0.136464	4.553773	-1.154298
6	-1.259364	4.900418	-0.391387
6	0.037802	4.792581	1.646076
6	-1.176060	5.014112	0.995837
1	-2.202402	5.087560	-0.898376
1	0.103013	4.895346	2.726042
1	-2.057092	5.285650	1.571286
6	4.558287	1.808240	-2.869482
6	4.406773	1.546018	-4.243356
6	5.476878	1.114738	-2.061031
6	5.203564	0.539765	-4.804314
6	6.247043	0.112724	-2.665962
6	6.113461	-0.173451	-4.023969
1	5.107661	0.322246	-5.864848
1	6.964557	-0.435921	-2.061563
1	6.725645	-0.948440	-4.477524
6	-0.234843	4.440857	-2.655850

1	0.548884	5.016867	-3.161444
1	-0.135887	3.399703	-2.985933
1	-1.204468	4.810046	-3.002600
1	4.755378	1.133401	-0.021235
6	5.643282	1.427500	-0.594168
1	6.501594	0.887387	-0.183563
1	5.801548	2.498302	-0.420436
6	3.430673	2.316731	-5.099247
1	3.676426	3.384892	-5.137800
1	3.439534	1.935276	-6.124462
1	2.406210	2.237410	-4.717247
6	-0.076305	-0.193758	3.095257
1	0.190805	0.062506	4.126269
1	-0.697304	0.618255	2.697302
6	1.188058	4.444851	0.925939
6	2.500341	4.218986	1.637023
1	2.854016	3.188524	1.513195
1	3.289489	4.877933	1.255537
1	2.391946	4.409949	2.708797
6	0.736729	-0.800491	-0.361814
79	1.673597	0.951261	-1.019659
79	0.072099	-1.658348	-2.105397
6	-0.602581	-2.404349	-3.921582
6	-1.810886	-2.695408	-5.823064
1	-2.591352	-2.482245	-6.536880
6	-0.840009	-3.641973	-5.811471
1	-0.598107	-4.423759	-6.514533
7	-1.652681	-1.947189	-4.659974
7	-0.110642	-3.452843	-4.640769
6	1.008732	-4.277231	-4.247190
6	2.310915	-3.834904	-4.539435
6	0.748951	-5.503857	-3.608621
6	3.378574	-4.655435	-4.151620
6	1.848419	-6.289655	-3.239395
6	3.151638	-5.869380	-3.504213
1	4.394206	-4.334792	-4.367903
1	1.673150	-7.240314	-2.742638
1	3.992235	-6.493432	-3.212529
6	-2.504344	-0.838854	-4.294563
6	-2.160364	0.449885	-4.739598
6	-3.660445	-1.098720	-3.536933
6	-3.008916	1.506835	-4.385123
6	-4.477351	-0.009456	-3.205864
6	-4.154963	1.281372	-3.623114
1	-2.765520	2.512139	-4.718528
1	-5.376935	-0.184116	-2.621465
1	-4.802944	2.113235	-3.360078
6	-0.920166	0.701204	-5.561966
1	-0.011671	0.460344	-4.997028
1	-0.903061	0.092569	-6.474056
1	-0.864822	1.752943	-5.857849
6	-4.016469	-2.492166	-3.078671
1	-4.009745	-3.210548	-3.906556
1	-3.306224	-2.859883	-2.327607
1	-5.013638	-2.503448	-2.628723
6	-0.657574	-5.973828	-3.326421
1	-1.228450	-5.232686	-2.755758
1	-1.214554	-6.163657	-4.252366
1	-0.641254	-6.904851	-2.752230
6	2.566407	-2.524933	-5.243250
1	1.967744	-2.430365	-6.156963
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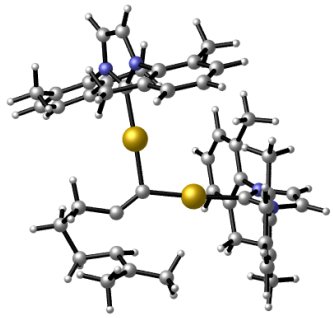
1	3.621734	-2.440320	-5.516981

Vb



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1	1.926010	-1.031712	2.653136
1	1.653922	0.537326	1.894235
6	-0.834874	-1.535558	2.968121
1	-0.528680	-2.232384	3.754043
1	-1.912407	-1.380985	3.079381
6	-0.549465	-2.143300	1.575828
1	-1.399370	-2.118829	0.896416
6	0.224488	-3.333977	1.455033
6	1.275219	-3.755895	2.425777
1	0.995685	-4.743784	2.822221
1	2.234110	-3.901254	1.910160
1	1.417475	-3.077537	3.266481
6	0.004312	-4.207947	0.279631
1	0.062238	-3.591749	-0.642737
1	0.722386	-5.029519	0.211695
1	-1.017473	-4.611316	0.293595
6	2.608688	2.717734	-1.561180
7	2.239009	3.982540	-1.209428
7	3.766923	2.884046	-2.260664
6	4.112756	4.230479	-2.342866
1	5.001920	4.561367	-2.856869
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1	3.026272	5.977776	-1.502876
6	1.063555	4.326269	-0.442389
6	-0.143356	4.559589	-1.125054
6	-1.265972	4.904588	-0.360975
6	0.033782	4.799868	1.674923
6	-1.181240	5.019080	1.026087
1	-2.209934	5.089824	-0.866954
1	0.100112	4.903065	2.754781
1	-2.062056	5.289363	1.602464
6	4.549545	1.823852	-2.852591
6	4.392533	1.562951	-4.226049
6	5.470955	1.129200	-2.048392
6	5.186209	0.556484	-4.790989
6	6.238255	0.127344	-2.657192
6	6.098806	-0.157876	-4.014834
1	5.085577	0.339454	-5.851188
1	6.957939	-0.422196	-2.056179
1	6.708520	-0.933039	-4.471422
6	-0.243469	4.445945	-2.626426
1	0.538544	5.023290	-3.133173
1	-0.142875	3.404865	-2.956142
1	-1.214282	4.813033	-2.972123
1	4.756351	1.146092	-0.006207
6	5.642475	1.440448	-0.581796

1	6.502033	0.899710	-0.174608
1	5.801488	2.511056	-0.407550
6	3.413394	2.335155	-5.077079
1	3.658037	3.403655	-5.113193
1	3.419642	1.956618	-6.103408
1	2.390105	2.253772	-4.692357
6	-0.044582	-0.215433	3.082906
1	0.233460	0.006842	4.118893
1	-0.649595	0.620972	2.711931
6	1.183781	4.453798	0.953547
6	2.497225	4.230514	1.663294
1	2.853500	3.201171	1.537961
1	3.284315	4.892036	1.282019
1	2.389178	4.419918	2.735382
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79	1.668210	0.954346	-1.007273
79	0.065879	-1.663651	-2.120408
6	-0.605975	-2.407778	-3.942256
6	-1.804321	-2.690563	-5.851667
1	-2.578408	-2.471595	-6.570657
6	-0.842139	-3.645830	-5.832420
1	-0.602461	-4.430519	-6.533024
7	-1.647048	-1.942445	-4.688294
7	-0.118771	-3.461568	-4.657167
6	0.992130	-4.294066	-4.256698
6	2.299247	-3.861765	-4.542146
6	0.719814	-5.518408	-3.618861
6	3.358679	-4.689575	-4.147282
6	1.811444	-6.311937	-3.242904
6	3.119212	-5.901275	-3.500204
1	4.377831	-4.376524	-4.358051
1	1.626446	-7.261099	-2.746799
1	3.953525	-6.531168	-3.203076
6	-2.492152	-0.827048	-4.329236
6	-2.135722	0.458395	-4.774126
6	-3.654822	-1.076803	-3.578302
6	-2.978462	1.522309	-4.426686
6	-4.465460	0.019165	-3.253932
6	-4.130864	1.306809	-3.671421
1	-2.725283	2.525225	-4.760089
1	-5.369803	-0.147744	-2.674659
1	-4.774152	2.143994	-3.413796
6	-0.887812	0.699467	-5.587736
1	0.014692	0.456397	-5.014224
1	-0.866428	0.086841	-6.497032
1	-0.824565	1.749652	-5.887519
6	-4.024621	-2.466675	-3.119945
1	-4.016845	-3.186847	-3.946274
1	-3.322954	-2.838183	-2.362672
1	-5.025330	-2.469572	-2.677794
6	-0.691560	-5.977678	-3.343051
1	-1.257693	-5.234135	-2.770749
1	-1.247670	-6.158699	-4.271234
1	-0.684922	-6.911165	-2.772607
6	2.568299	-2.555031	-5.246970
1	1.977243	-2.459386	-6.165522
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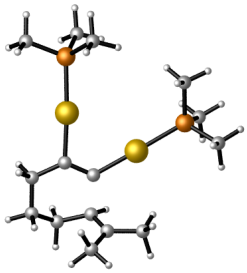

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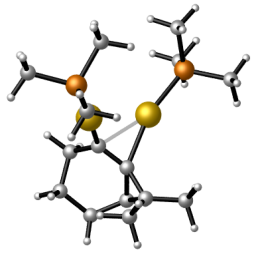
6	4.299143	2.358193	4.912325
1	4.684742	2.388718	5.939993
1	4.720752	3.229479	4.395856
6	2.781572	2.548040	4.957901
1	2.491644	3.597448	5.004643
6	1.939199	1.719272	5.725733
6	2.285683	0.336958	6.182773
1	1.578664	-0.005338	6.943916
1	2.233993	-0.372792	5.346555
1	3.300371	0.286654	6.590941
6	0.592810	2.211624	6.126058
1	-0.180826	1.454313	5.943352
1	0.611305	2.378481	7.215205
1	0.318931	3.150579	5.639098
79	2.239813	1.590206	0.516876
15	1.603967	1.558727	-1.756630
6	2.773700	0.619466	-2.818273
1	2.818407	-0.421655	-2.482649
1	2.453653	0.647172	-3.865959
1	3.775816	1.052623	-2.736013
6	1.512079	3.217290	-2.545324
1	1.260784	3.130401	-3.608525
1	0.750407	3.823883	-2.044993
1	2.477612	3.723915	-2.444846
6	-0.030867	0.791348	-2.100981
1	-0.816372	1.341746	-1.573362
1	-0.245575	0.799577	-3.175584
1	-0.030992	-0.243045	-1.741992
6	4.784343	1.085678	4.207242
1	4.445821	0.194102	4.741777
1	5.880633	1.060438	4.232875
6	2.915778	1.567101	2.507999
6	2.051539	2.149060	3.341353
79	0.195630	2.926891	2.850847
15	-1.894997	3.830203	2.253946
6	-3.264870	3.342812	3.379173
1	-3.021663	3.636151	4.405605
1	-4.201597	3.826501	3.080244
1	-3.396838	2.256256	3.351946
6	-1.941985	5.668074	2.263210
1	-1.205318	6.060630	1.554656
1	-2.937931	6.030578	1.984855
1	-1.691295	6.037609	3.262865
6	-2.504197	3.373711	0.581082
1	-2.586770	2.284934	0.504264
1	-3.485968	3.822230	0.391947
1	-1.797093	3.728683	-0.175075

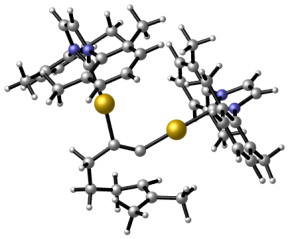
VIa



E = -1544.477572 h.
G = -1544.112121 h.

6	3.653965	3.218412	2.888041
1	4.196372	3.468710	1.971710
1	3.427065	4.159555	3.407614
6	3.856525	2.075576	5.192393
1	4.249608	1.149964	5.633605
1	4.143485	2.885730	5.873305
6	2.321981	2.059773	5.140350
1	1.834067	2.625914	5.932442
6	1.404194	0.899832	4.616030
6	2.000202	-0.446403	4.240857
1	1.356890	-0.971662	3.523095
1	2.991396	-0.345339	3.787501
1	2.091602	-1.083751	5.130302
6	0.046479	0.806291	5.296455
1	-0.689110	0.334017	4.632002
1	0.110096	0.198957	6.208274
1	-0.337128	1.794726	5.572155
79	2.028460	1.515708	0.767431
15	1.685684	0.477937	-1.332367
6	3.107383	0.654386	-2.483632
1	4.005946	0.225891	-2.027907
1	2.904954	0.140679	-3.430110
1	3.292373	1.715171	-2.681859
6	0.247585	1.110041	-2.288314
1	0.158752	0.582568	-3.244748
1	-0.671773	0.964470	-1.711870
1	0.372757	2.180885	-2.479179
6	1.400844	-1.335307	-1.235681
1	0.502862	-1.535426	-0.642053
1	1.272945	-1.760789	-2.237374
1	2.253292	-1.817526	-0.746337
6	4.526986	2.328693	3.816172
1	4.712708	1.376814	3.301648
1	5.506365	2.799109	3.965513
6	2.392559	2.401260	2.606767
6	1.736053	2.084272	3.782714
79	0.346705	3.597254	2.862301
15	-1.442533	5.056968	2.468252
6	-2.982819	4.546571	3.324581
1	-2.807868	4.508428	4.404399
1	-3.789321	5.257850	3.114655
1	-3.282209	3.550316	2.983436
6	-1.135267	6.777183	3.027457
1	-0.264440	7.184889	2.504247
1	-2.008882	7.405379	2.820112
1	-0.931747	6.783844	4.102934
6	-1.907649	5.207407	0.699307
1	-2.190193	4.225177	0.307714
1	-2.750678	5.898090	0.585087
1	-1.054307	5.581571	0.124971

$TS_{IVb-VIb}$

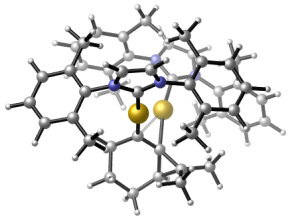


E = -2313.389348 h.
G = -2312.597424 h.

6	1.047363	-0.453576	0.628622
6	1.294397	-0.211314	2.111232
1	2.331202	-0.506982	2.333185
1	1.275826	0.872121	2.270259
6	-0.915157	-1.477310	2.468300
1	-1.494676	-2.038459	3.215242
1	-1.565240	-0.665733	2.119563
6	-0.668505	-2.389276	1.278533
1	-1.568183	-2.549254	0.687467
6	0.244631	-3.443162	1.204146
6	1.440611	-3.655259	2.091298
1	2.102713	-4.415137	1.665516
1	2.025038	-2.748547	2.254258
1	1.112039	-4.015749	3.076333
6	0.035861	-4.520958	0.186860
1	0.926459	-4.646908	-0.441643
1	-0.105009	-5.473765	0.720145
1	-0.835035	-4.344035	-0.447159
6	2.766671	2.678234	-1.495307
7	2.340271	3.971347	-1.425384
7	3.952457	2.746236	-2.164035
6	4.258076	4.060633	-2.506525
1	5.160813	4.314951	-3.040092
6	3.243469	4.831023	-2.042686
1	3.075580	5.895916	-2.089821
6	1.120525	4.418006	-0.792097
6	-0.045549	4.510495	-1.572071
6	-1.211098	4.971665	-0.946635
6	-0.032145	5.240479	1.146878
6	-1.207182	5.329345	0.401157
1	-2.124944	5.053425	-1.529129
1	-0.028621	5.531664	2.193964
1	-2.119551	5.689498	0.869041
6	4.813291	1.628915	-2.477769
6	4.755533	1.080889	-3.771683
6	5.712773	1.170682	-1.497873
6	5.631003	0.028827	-4.070815
6	6.561661	0.110256	-1.841582
6	6.522740	-0.456545	-3.114864
1	5.610282	-0.405939	-5.066533
1	7.266009	-0.260941	-1.101790
1	7.194805	-1.272856	-3.365842
6	-0.056715	4.126348	-3.031302
1	0.772014	4.585204	-3.582306
1	0.031608	3.040387	-3.157616
1	-0.992237	4.443956	-3.500838
1	4.865093	1.600754	0.447230
6	5.781566	1.792063	-0.124261
1	6.622338	1.377577	0.439764
1	5.910176	2.879835	-0.175288

6	3.789009	1.593929	-4.812133
1	3.944462	2.658220	-5.025833
1	3.910435	1.044999	-5.750400
1	2.748198	1.481599	-4.485837
6	0.333276	-0.887290	3.125362
1	0.855009	-1.661092	3.694183
1	0.013426	-0.140052	3.860996
6	1.158220	4.785168	0.565264
6	2.423467	4.692747	1.383043
1	2.707339	3.647936	1.560455
1	3.271157	5.177307	0.885421
1	2.284393	5.170553	2.357424
6	0.364089	-1.415511	0.011425
79	1.867337	1.056891	-0.572453
79	-0.187506	-1.857751	-1.920699
6	-0.812510	-2.313101	-3.837476
6	-2.009270	-2.380319	-5.766677
1	-2.793346	-2.093748	-6.450226
6	-1.015420	-3.296306	-5.875083
1	-0.751153	-3.971526	-6.674090
7	-1.872266	-1.787775	-4.515126
7	-0.293859	-3.245593	-4.686676
6	0.837049	-4.098505	-4.402901
6	2.133557	-3.578242	-4.557822
6	0.593963	-5.431228	-4.021372
6	3.212456	-4.430804	-4.288749
6	1.704405	-6.245619	-3.765013
6	3.002170	-5.750892	-3.892682
1	4.224230	-4.050385	-4.400202
1	1.541469	-7.277900	-3.466663
1	3.851440	-6.398106	-3.690737
6	-2.763275	-0.763920	-4.018346
6	-2.528207	0.570238	-4.396018
6	-3.855420	-1.146805	-3.218954
6	-3.421574	1.543466	-3.930285
6	-4.718698	-0.136952	-2.773499
6	-4.504409	1.195521	-3.123259
1	-3.264555	2.581235	-4.211279
1	-5.570779	-0.407615	-2.155434
1	-5.188228	1.964058	-2.772991
6	-1.357963	0.954517	-5.268873
1	-0.402437	0.727587	-4.781128
1	-1.365932	0.416442	-6.224136
1	-1.379541	2.025874	-5.488009
6	-4.102011	-2.586558	-2.839986
1	-4.057713	-3.253076	-3.708871
1	-3.354007	-2.942580	-2.120525
1	-5.087553	-2.696652	-2.377921
6	-0.805142	-5.984282	-3.892798
1	-1.426387	-5.374875	-3.226700
1	-1.318008	-6.022969	-4.861583
1	-0.776549	-7.001488	-3.491318
6	2.373551	-2.152410	-4.988799
1	1.755431	-1.875679	-5.850510
1	2.138057	-1.450796	-4.179206
1	3.423135	-2.010809	-5.260575

VIb

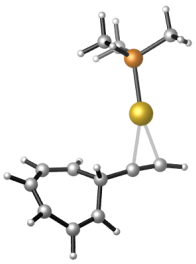


E = -2313.424020 h.
G = -2312.629026 h.

6	0.239489	-0.548099	-0.078024
6	-1.045875	-0.311412	0.717728
1	-1.401446	0.719501	0.632195
1	-1.861340	-0.972787	0.394809
6	-0.335051	-2.146381	2.380658
1	0.296262	-2.272757	3.270715
1	-1.263151	-2.694078	2.584937
6	0.304811	-2.795515	1.145498
1	-0.086606	-3.781156	0.896956
6	1.782379	-2.619972	0.657245
6	2.787314	-1.864894	1.510863
1	3.598458	-1.462580	0.890769
1	2.329058	-1.025809	2.043402
1	3.241300	-2.535828	2.252519
6	2.372986	-3.825733	-0.056575
1	3.163753	-3.515860	-0.752553
1	2.817046	-4.524984	0.664112
1	1.615526	-4.366532	-0.632670
6	2.571409	2.664557	-1.233368
7	2.310230	3.974977	-0.964947
7	3.793536	2.676618	-1.836150
6	4.286861	3.973479	-1.940474
1	5.244163	4.185251	-2.391424
6	3.353047	4.790732	-1.392664
1	3.329047	5.861737	-1.263615
6	1.114754	4.473009	-0.322744
6	0.030649	4.863268	-1.129782
6	-1.108804	5.365271	-0.487906
6	-0.063742	5.093838	1.675251
6	-1.158214	5.477941	0.901345
1	-1.959521	5.674229	-1.089502
1	-0.099948	5.191809	2.757004
1	-2.048572	5.875360	1.381293
6	4.501949	1.509800	-2.310247
6	4.323284	1.110169	-3.646791
6	5.372854	0.845624	-1.428098
6	5.036678	-0.011727	-4.089394
6	6.061949	-0.272788	-1.915242
6	5.894448	-0.700550	-3.232033
1	4.918048	-0.338123	-5.119191
1	6.741100	-0.802505	-1.252516
1	6.442241	-1.566584	-3.593882
6	0.074887	4.746809	-2.634062
1	0.968382	5.221017	-3.056258
1	0.084232	3.697550	-2.953431
1	-0.802927	5.224081	-3.079781
1	4.646440	1.240205	0.575019
6	5.572685	1.312270	-0.006769
1	6.331879	0.702765	0.492045
1	5.898957	2.358452	0.034183
6	3.404968	1.855550	-4.584569
1	3.665710	2.918463	-4.651113
1	3.461862	1.432265	-5.591813

1	2.360836	1.801634	-4.254223
6	-0.682080	-0.646817	2.190745
1	0.168330	-0.018353	2.485792
1	-1.515198	-0.374781	2.850468
6	1.097395	4.584117	1.079227
6	2.271364	4.163759	1.929559
1	2.381937	3.072037	1.942616
1	3.216314	4.579676	1.562378
1	2.132800	4.496629	2.962443
6	0.655426	-1.867148	0.041548
79	1.399358	1.032828	-0.720558
79	-0.131591	-1.904743	-2.026450
6	-0.847721	-2.449757	-3.876333
6	-2.096340	-2.531882	-5.764556
1	-2.844106	-2.198040	-6.467062
6	-1.269697	-3.607035	-5.776968
1	-1.147073	-4.406092	-6.491781
7	-1.826016	-1.832259	-4.592972
7	-0.510907	-3.542938	-4.612539
6	0.486854	-4.526873	-4.256163
6	1.808565	-4.333457	-4.696339
6	0.084092	-5.659409	-3.525009
6	2.750831	-5.315950	-4.366278
6	1.062817	-6.615000	-3.221492
6	2.383889	-6.444705	-3.634321
1	3.778953	-5.191562	-4.695465
1	0.778479	-7.500384	-2.659229
1	3.128000	-7.198672	-3.392299
6	-2.501636	-0.612543	-4.211772
6	-2.032659	0.603864	-4.740312
6	-3.619120	-0.694237	-3.362074
6	-2.717662	1.772155	-4.382664
6	-4.268994	0.502311	-3.030662
6	-3.821760	1.724205	-3.531717
1	-2.378606	2.724299	-4.781569
1	-5.137730	0.466456	-2.378801
1	-4.342978	2.640760	-3.268634
6	-0.848225	0.661963	-5.673919
1	0.044546	0.212242	-5.224199
1	-1.042314	0.123681	-6.609899
1	-0.613352	1.699714	-5.928084
6	-4.121296	-2.012044	-2.823736
1	-4.205689	-2.769349	-3.611243
1	-3.447601	-2.415852	-2.057459
1	-5.106908	-1.886235	-2.365835
6	-1.342258	-5.852444	-3.068882
1	-1.614692	-5.129622	-2.289512
1	-2.057668	-5.727323	-3.889575
1	-1.476880	-6.855328	-2.653062
6	2.212394	-3.118747	-5.495988
1	1.561079	-2.966684	-6.364488
1	2.163723	-2.205780	-4.889888
1	3.239399	-3.224124	-5.857955

IXa

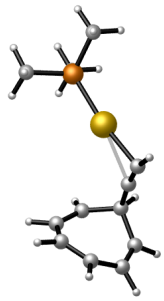


E = -944.456333 h.

G = -944.250497 h.

6	1.560353	2.642483	-1.041103
6	2.289681	3.028266	1.257459
6	0.431535	3.380771	-1.127782
1	2.221339	2.521617	-1.894910
6	1.343466	3.861457	1.746746
1	3.328951	3.115065	1.563503
6	-0.424800	3.741808	-0.019992
1	0.148909	3.769047	-2.105397
6	-0.017844	3.955536	1.269016
1	1.628061	4.550695	2.540833
1	-1.452637	4.000998	-0.267915
1	-0.747814	4.371639	1.961130
6	2.961634	0.937297	0.071329
6	3.835179	0.120143	-0.213978
1	4.562048	-0.498254	-0.707640
6	1.911676	1.945776	0.262969
1	1.010247	1.432828	0.631857
15	3.920257	-0.974030	4.206473
79	3.697162	-0.234877	2.016605
6	2.362306	-0.827151	5.158086
1	1.575901	-1.408742	4.667177
1	2.506900	-1.200781	6.177690
1	2.051549	0.221392	5.197652
6	5.184224	-0.061960	5.167362
1	4.927538	1.001295	5.201205
1	5.235980	-0.455598	6.188455
1	6.161359	-0.173224	4.687059
6	4.397636	-2.739815	4.305759
1	5.361610	-2.890423	3.809936
1	4.477117	-3.047578	5.354214
1	3.642874	-3.353570	3.804739

Xa

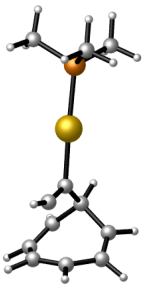


E = -944.456024 h.
G = -944.250409 h.

6	-1.263378	1.485006	-1.594073
1	-2.289914	1.657168	-1.861942
6	-0.074211	1.634508	-1.310690
6	1.338362	1.976325	-1.029514
6	1.505344	3.488436	-0.993178
6	1.873830	1.388809	0.264760
1	1.929827	1.581471	-1.861385
6	0.929182	4.284936	-0.064896
1	2.101538	3.925913	-1.789366
6	1.388798	1.688870	1.491398
1	2.698814	0.687551	0.167933
6	0.214811	3.867760	1.120240
1	1.028557	5.361024	-0.203175
6	0.419042	2.710246	1.815195
1	1.789640	1.130430	2.336854
1	-0.451511	4.606079	1.562301
1	-0.094384	2.601089	2.768774
79	-0.769519	-0.662575	-1.176625

15	-0.750493	-2.968866	-0.887686
6	-1.098542	-3.501348	0.830180
1	-2.085770	-3.140279	1.135000
1	-1.076962	-4.594933	0.893810
1	-0.347022	-3.083993	1.507557
6	-1.994376	-3.819253	-1.929649
1	-1.796005	-3.610417	-2.985379
1	-1.949234	-4.900526	-1.758843
1	-2.996113	-3.455988	-1.680078
6	0.859474	-3.725269	-1.324177
1	0.817937	-4.810210	-1.176846
1	1.096217	-3.510636	-2.370964
1	1.647535	-3.305182	-0.691647

$TS_{Xa\text{-}XIa}$



E = -944.437226 h.
G = -944.230065 h.

6	-0.840504	1.664659	0.300164
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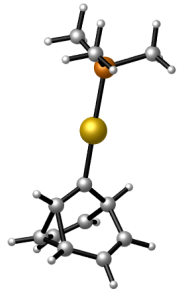
6	0.217878	1.024127	0.004427
6	1.659137	1.566972	-0.004071
6	1.784274	2.756993	-0.928844
6	2.035065	2.125207	1.350476
1	2.357821	0.785868	-0.297753
6	0.904629	3.785509	-0.891851
1	2.586068	2.736976	-1.662332
6	1.223281	2.975993	2.021039
1	2.966558	1.780375	1.791221
6	-0.109259	3.932883	0.119117
1	0.938904	4.545486	-1.669593
6	0.035515	3.559400	1.453796
1	1.455046	3.235377	3.051730
1	-0.978726	4.538029	-0.129492
1	-0.731287	3.902942	2.144980
79	-0.273988	-0.969424	-0.518324
15	-0.696197	-3.183967	-1.131989
6	-0.969097	-4.310431	0.290387
1	-1.842105	-3.978043	0.860804
1	-1.137562	-5.333700	-0.063494
1	-0.094420	-4.295883	0.948214
6	-2.183496	-3.382723	-2.187574
1	-2.057905	-2.809486	-3.111480
1	-2.335407	-4.439148	-2.435025
1	-3.064769	-3.006338	-1.658785
6	0.670599	-3.946541	-2.088990
1	0.421154	-4.981541	-2.348192
1	0.840029	-3.375852	-3.007446
1	1.590018	-3.935574	-1.494993

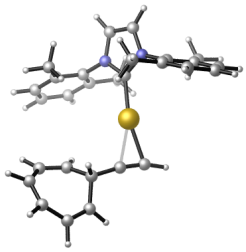
XIa



E = -944.466027 h.
G = -944.255582h.

6	-0.662884	1.988684	0.324270
1	-1.722645	1.766454	0.333509
6	0.296915	1.025064	0.006742
6	1.719428	1.511899	0.044915
6	1.893830	2.732822	-0.873337
6	2.041333	2.145205	1.407473
1	2.432057	0.727372	-0.204141
6	0.916118	3.645777	-0.922837
1	2.838902	2.835050	-1.397129
6	1.106699	2.892415	2.008094
1	3.045488	2.012253	1.797312
6	-0.283880	3.497203	-0.084936
1	0.994779	4.542379	-1.531395
6	-0.190457	3.127622	1.355309
1	1.287189	3.387213	2.958489
1	-1.169090	4.060850	-0.364863
1	-1.016558	3.461078	1.976616
79	-0.169399	-0.897760	-0.507502
15	-0.690229	-3.125187	-1.127083
6	-0.902604	-4.254033	0.305532
1	-1.708431	-3.887997	0.949414
1	-1.146368	-5.265818	-0.037209
1	0.022741	-4.285860	0.889573
6	-2.245681	-3.287584	-2.087798
1	-2.168213	-2.712109	-3.015670
1	-2.437741	-4.338382	-2.330854
1	-3.083008	-2.894650	-1.502423
6	0.593728	-3.923455	-2.168184
1	0.300979	-4.948200	-2.422458
1	0.730285	-3.349037	-3.090004
1	1.544190	-3.945121	-1.625538

IXb

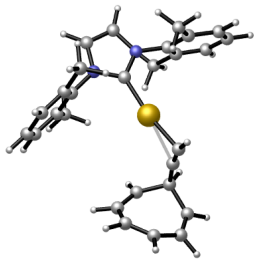


E = -1328.931381 h.
G = -1328.511295 h.

6	1.332524	1.948556	-0.454710
6	1.637531	2.975889	1.739603
6	0.099475	2.367714	-0.816447
1	2.117588	1.804918	-1.192160
6	0.480965	3.650167	1.930189

1	2.581562	3.362111	2.114660
6	-0.959322	2.748110	0.092045
1	-0.117779	2.460154	-1.879878
6	-0.789358	3.321955	1.322899
1	0.503064	4.537208	2.561966
1	-1.973640	2.701885	-0.300468
1	-1.679388	3.695047	1.826691
6	2.887700	0.895361	1.153049
6	3.951578	0.276619	1.094301
1	4.845121	-0.224817	0.770433
6	1.633842	1.648929	1.003816
1	0.814441	1.032155	1.403602
79	3.585811	0.295797	3.289040
6	3.700247	0.038235	5.303646
6	3.832877	0.420809	7.524491
1	3.870343	1.017818	8.422432
6	3.866478	-0.924428	7.339036
1	3.939627	-1.740017	8.041921
7	3.732369	0.997554	6.264537
7	3.782646	-1.143149	5.969869
6	3.789525	-2.450364	5.349227
6	5.028940	-3.049034	5.057368
6	2.557889	-3.078106	5.089972
6	5.009394	-4.315880	4.459818
6	2.591598	-4.344207	4.490756
6	3.803836	-4.957023	4.176057
1	5.952763	-4.800797	4.223356
1	1.654221	-4.851811	4.279761
1	3.809560	-5.941317	3.715804
6	3.675385	2.421649	6.018263
6	4.875547	3.104817	5.751869
6	2.426319	3.065688	6.081763
6	4.795625	4.484555	5.521271
6	2.399364	4.446103	5.845288
6	3.570491	5.148994	5.563131
1	5.708116	5.037608	5.314932
1	1.447983	4.969122	5.890075
1	3.529397	6.220258	5.385621
6	1.153347	2.316175	6.393986
1	0.924384	1.567178	5.626341
1	1.216173	1.785906	7.351398
1	0.307915	3.007909	6.448081
6	6.208019	2.396105	5.709939
1	6.356783	1.750737	6.582946
1	6.298122	1.761491	4.819162
1	7.024657	3.123248	5.683790
6	1.239402	-2.425131	5.427237
1	1.229869	-2.022563	6.446293
1	1.018594	-1.592536	4.747101
1	0.423655	-3.148906	5.340972
6	6.340755	-2.365499	5.360224
1	6.479102	-1.466906	4.746172
1	6.407936	-2.052681	6.408458
1	7.177335	-3.039626	5.155530

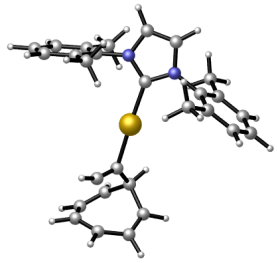
Xb



E = -1328.931004 h.
G = -1328.512940 h.

6	-1.766994	-0.228129	-0.781939
1	-2.828340	-0.375293	-0.864236
6	-0.641504	0.272296	-0.712954
6	0.603763	1.077009	-0.669283
6	0.276016	2.553408	-0.830389
6	1.408216	0.885031	0.604398
1	1.216291	0.761650	-1.519428
6	-0.446480	3.265126	0.064101
1	0.630502	3.028500	-1.741217
6	0.955830	1.200171	1.839718
1	2.401893	0.460210	0.486787
6	-0.883910	2.832262	1.371761
1	-0.713100	4.285306	-0.210365
6	-0.259071	1.912087	2.163810
1	1.581107	0.920646	2.687084
1	-1.712168	3.387283	1.808206
1	-0.627546	1.795624	3.181261
79	-0.542597	-2.050865	-0.511151
6	0.085646	-3.977533	-0.326803
6	0.681255	-5.984441	0.518684
1	0.907031	-6.700656	1.293330
6	0.681666	-6.095829	-0.835261
1	0.905566	-6.930546	-1.481341
7	0.313688	-4.678198	0.814762
7	0.315440	-4.855087	-1.339581
6	0.205032	-4.545918	-2.748894
6	1.369470	-4.175449	-3.446015
6	-1.053646	-4.654233	-3.366692
6	1.240566	-3.885505	-4.810363
6	-1.130922	-4.351237	-4.732427
6	0.002796	-3.967702	-5.447700
1	2.124046	-3.596897	-5.373381
1	-2.091476	-4.428760	-5.234529
1	-0.076341	-3.740969	-6.507493
6	0.209798	-4.150050	2.158169
6	1.350989	-3.568837	2.739893
6	-1.015840	-4.272728	2.836785
6	1.232018	-3.082317	4.048275
6	-1.083841	-3.771279	4.143077
6	0.027012	-3.179279	4.743124
1	2.099207	-2.630709	4.522550
1	-2.018546	-3.854909	4.690989
1	-0.044094	-2.800586	5.759159
6	2.660950	-3.459854	1.997605
1	2.976336	-4.421154	1.576507
1	2.593298	-2.748288	1.165290
1	3.450766	-3.110667	2.669084
6	-2.222804	-4.917058	2.198691
1	-2.584731	-4.335516	1.341996
1	-2.002087	-5.926593	1.832870
1	-3.041404	-4.991861	2.920036
6	-2.285616	-5.080184	-2.605808
1	-3.117399	-5.252057	-3.295080
1	-2.117343	-6.003647	-2.039774
1	-2.600276	-4.312685	-1.887641
6	2.714598	-4.084510	-2.765967
1	2.729375	-3.297477	-2.002031
1	2.985690	-5.021812	-2.266424
1	3.496332	-3.855408	-3.495837

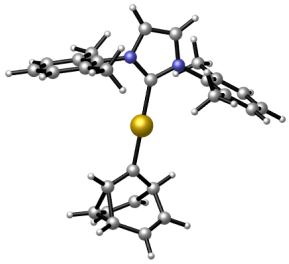
$TS_{Xb\text{-}XIb}$



E = -1328.911054 h.
G = -1328.490381 h.

6	-1.211560	0.362549	0.707438
1	-2.133273	0.192127	1.232420
6	-0.139159	0.042313	0.100712
6	0.910707	1.000675	-0.489025
6	0.285188	1.938139	-1.497811
6	1.452241	1.932289	0.572532
1	1.721546	0.438842	-0.948798
6	-0.858738	2.611453	-1.231461
1	0.765374	2.019091	-2.469329
6	0.633817	2.603408	1.416500
1	2.532140	2.010114	0.665500
6	-1.483200	2.641096	0.065637
1	-1.357985	3.154909	-2.030693
6	-0.799087	2.637544	1.279541
1	1.060840	3.142133	2.259632
1	-2.547224	2.865960	0.102945
1	-1.381226	2.859468	2.171662
79	-0.007646	-2.055985	0.009038
6	0.200443	-4.085656	-0.149841
6	0.420611	-6.284278	0.339103
1	0.504400	-7.148731	0.979447
6	0.417217	-6.166608	-1.013004
1	0.495475	-6.907094	-1.794036
7	0.287587	-4.998798	0.854240
7	0.282253	-4.811724	-1.296749
6	0.234121	-4.258562	-2.631972
6	1.447110	-3.965470	-3.282001
6	-1.021199	-4.057693	-3.233860
6	1.375475	-3.432919	-4.575592
6	-1.040423	-3.521405	-4.528234
6	0.144877	-3.208890	-5.192636
1	2.297459	-3.198516	-5.100893
1	-1.997516	-3.359193	-5.017035
1	0.110291	-2.798879	-6.198384
6	0.249397	-4.685929	2.265511
6	1.457104	-4.385453	2.920830
6	-0.990234	-4.721238	2.929338
6	1.395409	-4.092647	4.289622
6	-1.000337	-4.420290	4.297434
6	0.179310	-4.105973	4.971689
1	2.314678	-3.859680	4.820489
1	-1.945109	-4.441043	4.834027
1	0.151905	-3.879581	6.034195
6	2.778801	-4.366980	2.191515
1	2.930172	-5.273187	1.594273
1	2.847532	-3.512990	1.505950
1	3.605457	-4.288653	2.903593
6	-2.272851	-5.065109	2.210732
1	-2.534197	-4.304796	1.464424
1	-2.201727	-6.022898	1.682542
1	-3.100939	-5.133178	2.922017
6	-2.310821	-4.396529	-2.525809
1	-3.149482	-4.366050	-3.227407
1	-2.281019	-5.394972	-2.075665
1	-2.524638	-3.683611	-1.719446
6	2.785492	-4.202280	-2.623865
1	2.932627	-3.543041	-1.759342
1	2.888859	-5.231846	-2.262862
1	3.597787	-4.009859	-3.330777

XIb

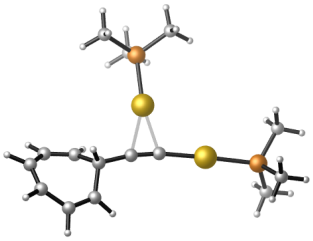


E = -1328.942491 h.
G = -1328.517135 h.

6	-0.712375	0.686448	1.180867
1	-1.151353	0.146038	2.010242
6	-0.101708	0.022539	0.107149
6	0.453066	0.932419	-0.956521
6	-0.637202	1.879277	-1.480179
6	1.435348	1.941583	-0.341892
1	0.917230	0.377972	-1.770534
6	-1.512979	2.396977	-0.609853
1	-0.610035	2.142847	-2.532762
6	1.146805	2.476920	0.850752
1	2.296210	2.230306	-0.936707
6	-1.411204	2.080786	0.824135
1	-2.284862	3.097183	-0.917067
6	-0.102310	2.120680	1.543361
1	1.786540	3.220658	1.317765
1	-2.286820	2.256799	1.442269
1	-0.163427	2.321242	2.609014
79	0.044807	-1.993418	-0.025405
6	0.207007	-4.050242	-0.166197
6	0.347127	-6.248292	0.358986
1	0.373245	-7.107019	1.012014
6	0.428803	-6.146461	-0.992924
1	0.536480	-6.898798	-1.758950
7	0.210247	-4.955231	0.849837
7	0.342749	-4.793462	-1.297836
6	0.391498	-4.251426	-2.637960
6	1.649766	-4.010126	-3.219832
6	-0.819016	-4.002571	-3.309230
6	1.672680	-3.478768	-4.515739
6	-0.743689	-3.470042	-4.603123
6	0.488382	-3.206909	-5.200495
1	2.632005	-3.283774	-4.987942
1	-1.664578	-3.269036	-5.144033
1	0.526141	-2.798052	-6.206604

6	0.099566	-4.624144	2.253488
6	1.272873	-4.321551	2.967479
6	-1.173683	-4.643230	2.851181
6	1.141181	-4.011625	4.327614
6	-1.253760	-4.325389	4.213173
6	-0.109123	-4.009692	4.944816
1	2.032849	-3.776310	4.902568
1	-2.225848	-4.332843	4.698854
1	-0.191007	-3.770084	6.001640
6	2.630358	-4.314296	2.307484
1	2.800084	-5.215426	1.707801
1	2.744026	-3.453550	1.636136
1	3.420582	-4.254452	3.061594
6	-2.418828	-4.985219	2.068965
1	-2.629498	-4.234559	1.297095
1	-2.330007	-5.952261	1.560633
1	-3.285714	-5.032598	2.734405
6	-2.159492	-4.285315	-2.674561
1	-2.954221	-4.234462	-3.424779
1	-2.192341	-5.278075	-2.212165
1	-2.394234	-3.555041	-1.889687
6	2.938158	-4.302223	-2.488729
1	3.044209	-3.680783	-1.591197
1	2.996852	-5.347520	-2.164066
1	3.796553	-4.102501	-3.136347

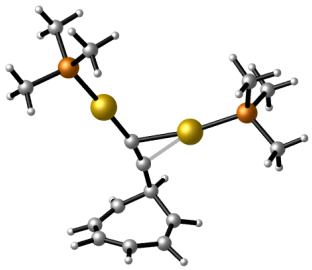
XIIa



E = -1540.832040 h.
G = -1540.535013 h.

6	1.625611	2.753369	-1.010189
6	2.122267	2.966216	1.359896
6	0.492172	3.476972	-1.154097
1	2.372840	2.717261	-1.798923
6	1.114962	3.743234	1.822051
1	3.125453	3.044704	1.771775
6	-0.475234	3.733294	-0.110979
1	0.295565	3.937907	-2.121487
6	-0.196742	3.851833	1.224381
1	1.305961	4.371479	2.691501
1	-1.481048	3.995834	-0.435235
1	-0.998984	4.201264	1.872243
6	2.945647	0.964865	0.091277
6	3.829879	0.162113	-0.257158
6	1.868107	1.954629	0.258410
1	0.937990	1.416742	0.501171
15	4.017673	-0.928853	4.173225
79	3.765179	-0.219342	1.980371
6	2.486927	-0.761643	5.167907
1	1.684174	-1.346676	4.708378
1	2.656450	-1.118678	6.189755
1	2.180089	0.288514	5.198609
6	5.304474	-0.016475	5.108064
1	5.057183	1.049421	5.133456
1	5.370995	-0.397341	6.133243
1	6.273434	-0.138966	4.613628
6	4.489179	-2.695873	4.309747
1	5.444209	-2.862137	3.801388
1	4.585568	-2.981552	5.363154
1	3.725184	-3.319122	3.834863
79	5.198853	-1.062365	-1.127642
15	6.762062	-2.433587	-2.203848
6	7.566584	-3.667603	-1.108015
1	8.287105	-4.267838	-1.674674
1	8.087269	-3.154047	-0.293461
1	6.808501	-4.329127	-0.676755
6	6.056946	-3.420576	-3.581149
1	5.614239	-2.751097	-4.325468
1	6.837951	-4.023398	-4.057530
1	5.273328	-4.081556	-3.197402
6	8.153544	-1.502787	-2.956706
1	8.854069	-2.190766	-3.442811
1	7.766823	-0.795903	-3.697522
1	8.681825	-0.939509	-2.180836

XIIIa

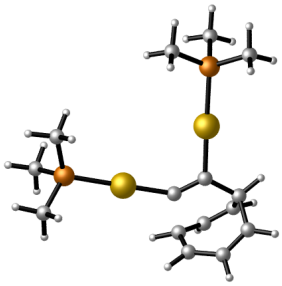


E = -1540.830824 h.
G = -1540.533971 h.

6	-0.449310	1.025217	0.674112
6	0.910509	1.422912	1.116519
6	1.933407	1.467025	-0.007165
6	0.881793	2.779226	1.805073
1	1.243899	0.679708	1.847525
6	1.875277	2.313561	-1.061209
1	2.752308	0.754123	0.059280
6	0.574014	3.940683	1.183747
1	1.098500	2.783320	2.870639
6	0.966893	3.423255	-1.235738
1	2.609997	2.174688	-1.854119
6	0.387785	4.148721	-0.234498
1	0.478218	4.828826	1.807820
1	0.843576	3.788231	-2.253834
1	-0.162017	5.044174	-0.518901
79	-0.817649	-1.082579	-0.378779
15	-0.401994	-3.181149	-1.275982
6	0.039287	-4.448837	-0.026516
1	-0.772819	-4.545712	0.700920
1	0.209182	-5.416519	-0.511600
1	0.947823	-4.145295	0.502915
6	-1.846850	-3.873183	-2.170017
1	-2.123258	-3.207859	-2.994026
1	-1.603625	-4.863482	-2.571178
1	-2.697918	-3.959686	-1.487432
6	0.968851	-3.207947	-2.493889
1	1.104177	-4.220372	-2.890543
1	0.742350	-2.524362	-3.318083
1	1.896337	-2.881188	-2.013446
6	-1.651980	0.869396	0.392473
79	-3.661938	0.941241	0.097244
15	-5.980090	1.097050	-0.189696
6	-6.947556	0.516245	1.258336

1	-8.021862	0.611242	1.064964
1	-6.710518	-0.532760	1.463234
1	-6.685707	1.110839	2.139406
6	-6.631606	0.127757	-1.606526
1	-7.716075	0.257574	-1.692419
1	-6.154158	0.463245	-2.532659
1	-6.406499	-0.933807	-1.462159
6	-6.560826	2.812546	-0.488512
1	-6.080213	3.210643	-1.387975
1	-7.648227	2.833034	-0.620374
1	-6.288653	3.446709	0.361304
1	-6.181235	2.194377	1.692146
6	-6.009153	-0.223010	-1.328359
1	-7.100740	-0.239585	-1.420962
1	-5.563205	-0.253763	-2.327741
1	-5.681331	-1.107827	-0.773349
6	-6.208063	2.670903	-1.419562
1	-5.759642	2.706622	-2.417628
1	-7.290102	2.528400	-1.516469
1	-6.014509	3.624113	-0.917112

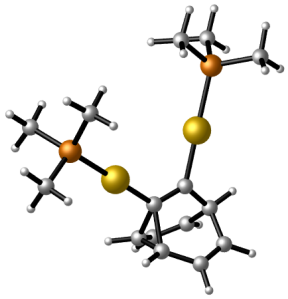
$TS_{XIIIa\text{-}XIVa}$



E = -1540.796996 h.
G = -1540.498535 h.

6	-0.013200	0.910398	-0.187384
6	1.415661	1.474628	-0.004500
6	1.740510	2.650740	-0.872734
6	1.523095	2.093750	1.393761
1	2.166538	0.694909	-0.130312
6	0.853603	3.670073	-1.066608
1	2.694115	2.651385	-1.395053
6	0.514030	2.859591	1.829717
1	2.416376	1.890330	1.976444
6	-0.363541	3.769133	-0.345881
1	1.050386	4.417849	-1.831128
6	-0.603529	3.201955	0.936585
1	0.488318	3.257777	2.840738
1	-1.170094	4.354479	-0.782632
1	-1.508239	3.554175	1.424610
79	-0.255586	-1.115952	-0.616458
15	-0.487581	-3.403180	-1.106835
6	-0.335575	-4.499213	0.359992
1	-1.119430	-4.253710	1.083724
1	-0.430416	-5.550960	0.067392
1	0.637481	-4.345741	0.837694
6	-2.103844	-3.856448	-1.852935
1	-2.242295	-3.307017	-2.789672
1	-2.145539	-4.932400	-2.056050
1	-2.915146	-3.588036	-1.168618
6	0.759133	-4.047581	-2.291616
1	0.592065	-5.113588	-2.482556
1	0.690718	-3.497356	-3.235404
1	1.764502	-3.909309	-1.880732
6	-1.101001	1.629401	0.039870
79	-3.136209	1.482557	-0.191117
15	-5.461837	1.296986	-0.454908
6	-6.397259	1.282242	1.126437
1	-7.474773	1.224224	0.935810
1	-6.090621	0.420133	1.727627

XIVa

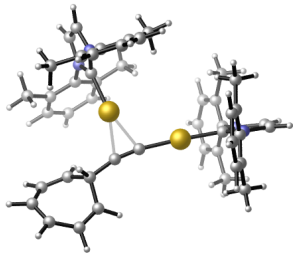


E = -1540.800786 h.
G = -1540.500099 h.

6	0.050462	1.026196	-0.148070
6	1.481644	1.482148	0.077171
6	1.840144	2.636405	-0.859251
6	1.618667	2.167984	1.438322
1	2.192759	0.661715	-0.021052
6	0.907820	3.568592	-1.103014
1	2.851898	2.685384	-1.250074
6	0.622536	2.965188	1.849462
1	2.539961	2.023806	1.994479
6	-0.400946	3.502457	-0.444785
1	1.096299	4.414865	-1.758648
6	-0.540008	3.207892	0.987822
1	0.655595	3.485720	2.803108
1	-1.204668	4.085355	-0.884185
1	-1.431780	3.604440	1.463555
79	-0.334799	-0.952837	-0.537336
15	-0.733989	-3.250967	-0.952005
6	-0.266084	-4.334006	0.455930
1	-0.841242	-4.052147	1.343939
1	-0.463730	-5.384976	0.217299
1	0.798323	-4.208275	0.678765
6	-2.484891	-3.683223	-1.304177
1	-2.825835	-3.140904	-2.192081
1	-2.588939	-4.759696	-1.480472
1	-3.113757	-3.395614	-0.455310
6	0.203637	-3.921499	-2.382429
1	-0.002216	-4.989886	-2.511932
1	-0.082051	-3.386489	-3.293894
1	1.276369	-3.778066	-2.217885
6	-0.965091	1.972263	-0.057688
79	-2.992393	1.579762	-0.343925
15	-5.285287	1.153789	-0.662051
6	-6.171668	0.643336	0.864942
1	-7.231681	0.460363	0.655717
1	-5.720737	-0.271630	1.262819

1	-6.086233	1.429770	1.621928
6	-5.661421	-0.177496	-1.871146
1	-6.743755	-0.312298	-1.975002
1	-5.236286	0.080573	-2.846464
1	-5.213402	-1.118078	-1.535023
6	-6.232499	2.603727	-1.276876
1	-5.822525	2.931035	-2.237910
1	-7.290815	2.350559	-1.405353
1	-6.144548	3.429215	-0.562989

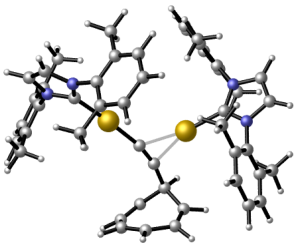
XIIb



E = -2309.780774 h.
G = -2309.056972 h.

6	2.419880	1.402832	-1.426335
6	2.273630	2.512288	0.731235
6	1.246074	1.720809	-2.018106
1	3.330493	1.295277	-2.010307
6	1.061630	3.113658	0.692327
1	3.111700	2.974794	1.246828
6	0.022512	2.055230	-1.324576
1	1.213230	1.763161	-3.106337
6	-0.060800	2.679821	-0.109007
1	0.916720	4.021402	1.277277
1	-0.902988	1.927641	-1.883936
1	-1.046477	3.009065	0.216247
6	3.740443	0.492170	0.467650
6	4.838517	-0.096473	0.511813
6	2.486646	1.163461	0.071224
1	1.640103	0.516201	0.348271
79	4.177447	0.080978	2.683527
6	4.010123	-0.007456	4.709072
6	4.048217	0.534282	6.904966
1	4.189667	1.176241	7.760620
6	3.669650	-0.766177	6.812718
1	3.413137	-1.489324	7.571185
7	4.253126	0.985453	5.606470
7	3.648662	-1.083095	5.459336
6	3.283174	-2.382673	4.938901
6	4.293646	-3.344647	4.759776
6	1.927319	-2.641141	4.668860
6	3.910969	-4.603277	4.278212
6	1.594903	-3.914466	4.188322
6	2.575656	-4.886003	3.992301
1	4.672011	-5.365802	4.135417
1	0.553866	-4.140822	3.974162
1	2.296786	-5.869670	3.624162
6	4.655500	2.332945	5.268327
6	6.027399	2.614221	5.143728
6	3.657272	3.310774	5.108652
6	6.391705	3.928088	4.821597
6	4.071665	4.610476	4.789776
6	5.424308	4.916463	4.642314
1	7.445521	4.172786	4.719212
1	3.320699	5.385521	4.662247
1	5.725951	5.931056	4.396290
6	2.191405	2.990402	5.273116
1	1.845950	2.275407	4.516780
1	1.977570	2.549822	6.254041
1	1.590364	3.898844	5.173958
6	7.078936	1.550881	5.346886
1	6.949771	1.027377	6.301455
1	7.040670	0.792871	4.555220
1	8.078688	1.994142	5.335601
6	0.855843	-1.597434	4.873441
1	0.921324	-1.127490	5.860993
1	0.929804	-0.795726	4.127890
1	-0.136677	-2.047273	4.777243
6	5.742443	-3.047809	5.061886
1	6.158016	-2.320056	4.353599
1	5.875773	-2.633687	6.067911
1	6.340024	-3.961229	4.990822
79	6.606723	-1.036482	0.250430
6	8.392159	-1.976679	-0.121449
6	9.929587	-3.474547	-0.846158
1	10.277082	-4.397628	-1.283644
6	10.604470	-2.402890	-0.358553
1	11.661379	-2.198560	-0.284395
7	8.575258	-3.198062	-0.692982
7	9.648146	-1.494153	0.082273
6	7.513481	-4.094858	-1.091518
6	6.978053	-3.976613	-2.386435
6	7.076924	-5.066843	-0.173070
6	5.956360	-4.864681	-2.748130
6	6.053114	-5.931303	-0.580732
6	5.494595	-5.830307	-1.854695
1	5.527022	-4.793703	-3.743869
1	5.699002	-6.691100	0.110918
1	4.702586	-6.511054	-2.154956
6	9.958401	-0.214734	0.679623
6	10.236031	-0.168850	2.057990
6	9.991985	0.925920	-0.142495
6	10.542602	1.078234	2.616830
6	10.301547	2.151111	0.463261
6	10.572071	2.228766	1.828833
1	10.764393	1.138923	3.678986
1	10.334859	3.047766	-0.149849
1	10.814785	3.187642	2.278992
6	7.466078	-2.933036	-3.361812
1	7.165091	-1.924521	-3.051216
1	8.558543	-2.932511	-3.449275
1	7.046276	-3.113610	-4.355872
6	7.676932	-5.184735	1.206941
1	8.763479	-5.327603	1.170142
1	7.488904	-4.284575	1.804329
1	7.243214	-6.036701	1.738619
6	9.695482	0.853725	-1.620827
1	9.972164	1.790507	-2.113582
1	10.240886	0.038346	-2.109153
1	8.627140	0.682633	-1.804163
6	10.202394	-1.408029	2.919362
1	9.203902	-1.861233	2.932376
1	10.899763	-2.174821	2.561887
1	10.473385	-1.162146	3.950179

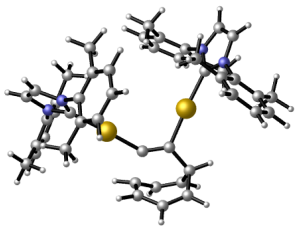
XIIIb



E = -2309.778750 h.
G = -2309.055188 h.

6	-0.306958	0.817808	0.388018
6	0.154531	0.701672	-1.055250
6	-0.761711	2.246353	0.640027
1	0.554176	0.617671	1.033056
6	-0.629958	0.939160	-2.132015
1	1.184958	0.389013	-1.208621
6	-1.764097	2.858465	-0.031682
1	-0.252248	2.779844	1.439142
6	-1.957309	1.508842	-2.133306
1	-0.214609	0.705981	-3.112135
6	-2.462260	2.365062	-1.196878
1	-2.070403	3.843722	0.319611
1	-2.552718	1.338207	-3.028758
1	-3.427551	2.822930	-1.406122
6	0.037689	-4.176885	0.421346
6	1.083342	-6.144705	0.814408
1	1.456621	-6.961104	1.413128
6	1.139488	-5.913512	-0.521951
1	1.572906	-6.485869	-1.327421
7	0.405277	-5.070404	1.378886
7	0.492984	-4.703947	-0.747431
6	0.344379	-4.095569	-2.050858
6	1.389092	-3.289004	-2.536579
6	-0.823075	-4.358931	-2.788292
6	1.229104	-2.716861	-3.805194
6	-0.936918	-3.764201	-4.052017
6	0.075943	-2.948307	-4.554872
1	2.021562	-2.089201	-4.204281
1	-1.828539	-3.952798	-4.644069
1	-0.029576	-2.498720	-5.538615
6	0.134289	-4.934866	2.792838
6	1.058214	-4.238781	3.592475
6	-1.026230	-5.534257	3.314004
6	0.778924	-4.133229	4.961273
6	-1.261193	-5.402048	4.688870
6	-0.370522	-4.705270	5.505107
1	1.477633	-3.601880	5.601824
1	-2.149258	-5.858456	5.117860
1	-0.567956	-4.616786	6.570047
6	2.306220	-3.617584	3.014173
1	2.865158	-4.325388	2.391478
1	2.066730	-2.751593	2.384115
1	2.968405	-3.273681	3.814289
6	-1.990909	-6.297814	2.439293
1	-2.476018	-5.643619	1.705163
1	-1.489554	-7.095494	1.878532
1	-2.774312	-6.757423	3.048623
6	-1.922654	-5.242646	-2.252440
1	-2.648128	-5.468710	-3.039417
1	-1.533001	-6.191799	-1.866865
1	-2.463113	-4.756010	-1.430920
6	2.643736	-3.042689	-1.734489
1	2.422717	-2.557378	-0.776341
1	3.172377	-3.976601	-1.508042
1	3.329530	-2.396103	-2.289288
6	-1.370853	-0.156958	0.754104
6	-2.417672	-0.739089	1.102565
79	-0.953051	-2.417058	0.684171
79	-4.271092	-1.284398	1.689568
6	-6.187834	-1.713159	2.278877
7	-6.946896	-0.985733	3.143993
7	-6.997924	-2.730342	1.876399
6	-8.214615	-1.540849	3.279573
1	-8.961843	-1.104237	3.924083
6	-8.247416	-2.637312	2.481422
1	-9.029430	-3.354415	2.285618
6	-6.637993	-3.772807	0.942220
6	-6.799366	-3.529699	-0.433821
6	-6.183653	-5.003581	1.450040
6	-6.472300	-4.566465	-1.317681
6	-5.874433	-6.010919	0.526804
6	-6.013185	-5.794969	-0.844179
1	-6.591040	-4.404242	-2.385620
1	-5.526815	-6.972877	0.893942
1	-5.773448	-6.590562	-1.544521
6	-6.516304	0.216268	3.822399
6	-6.765306	1.457908	3.210056
6	-5.896779	0.097165	5.079341
6	-6.361525	2.610611	3.895868
6	-5.509854	1.278455	5.725328
6	-5.737009	2.523577	5.139633
1	-6.544805	3.582251	3.444848
1	-5.030293	1.213568	6.698355
1	-5.433784	3.429205	5.658121
6	-7.438305	1.562748	1.862871
1	-6.806470	1.149431	1.066915
1	-8.388912	1.017593	1.835603
1	-7.641662	2.609507	1.618770
6	-5.649053	-1.246228	5.721528
1	-6.565548	-1.844675	5.783926
1	-4.917456	-1.833684	5.153166
1	-5.259278	-1.119034	6.735785
6	-6.021652	-5.246221	2.931585
1	-5.196629	-4.653766	3.346717
1	-6.923898	-4.981028	3.494063
1	-5.805294	-6.301334	3.123452
6	-7.302101	-2.206297	-0.957635
1	-8.198889	-1.869673	-0.425530
1	-6.544828	-1.419687	-0.847732
1	-7.546879	-2.284903	-2.021143

$TS_{XIIIb\text{-}XIVb}$



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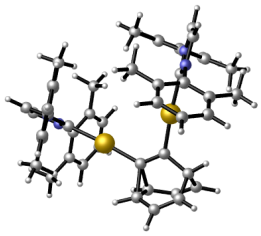
G = -2309.016648 h.

6	-0.439010	0.503407	-0.744147
6	-0.986039	1.193867	-1.957926
6	-0.179588	1.691283	0.189098

1	0.498809	0.004402	-0.986428
6	-2.254696	1.685846	-1.974749
1	-0.357796	1.252215	-2.843310
6	-1.225952	2.241369	0.818605
1	0.839900	2.050222	0.293670
6	-3.072482	1.706344	-0.810050
1	-2.692842	2.037745	-2.905739
6	-2.590702	1.774036	0.529867
1	-1.110410	3.042584	1.543896
1	-4.151386	1.734998	-0.943802
1	-3.344241	2.025511	1.271137
6	0.098030	-4.259927	0.615524
6	0.976628	-6.103667	1.604332
1	1.289475	-6.725236	2.429044
6	1.031821	-6.297722	0.262917
1	1.400853	-7.124233	-0.324512
7	0.402788	-4.851587	1.803927
7	0.491573	-5.159683	-0.327986
6	0.394955	-4.962911	-1.756373
6	1.473564	-4.358763	-2.427284
6	-0.758174	-5.413151	-2.423010
6	1.364121	-4.192595	-3.814193
6	-0.821971	-5.224590	-3.809687
6	0.226579	-4.617229	-4.499861
1	2.185041	-3.729385	-4.355236
1	-1.703773	-5.563623	-4.346658
1	0.160661	-4.481864	-5.576113
6	0.194467	-4.260373	3.106237
6	1.190175	-3.417026	3.631046
6	-0.978592	-4.581838	3.811952
6	0.972505	-2.868324	4.901699
6	-1.149484	-4.012383	5.080415
6	-0.186689	-3.159326	5.619474
1	1.727757	-2.213542	5.328259
1	-2.046512	-4.248326	5.646798
1	-0.335322	-2.728302	6.605989
6	2.452462	-3.098157	2.867494
1	2.927226	-3.999837	2.464497
1	2.247923	-2.432189	2.019948
1	3.175095	-2.596491	3.517935
6	-2.025976	-5.502940	3.235575
1	-2.487273	-5.074443	2.337598
1	-1.604564	-6.473485	2.948340
1	-2.818824	-5.683866	3.967456
6	-1.896303	-6.075205	-1.685759
1	-2.669507	-6.395768	-2.389877
1	-1.561831	-6.956866	-1.125878
1	-2.358935	-5.390712	-0.965153
6	2.709435	-3.893988	-1.695930
1	2.490459	-3.041221	-1.041441
1	3.134584	-4.683474	-1.065570
1	3.477737	-3.579185	-2.408089
6	-1.423614	-0.471839	-0.050165
6	-2.600020	-0.061127	0.423498
79	-0.717719	-2.388659	0.303200
79	-4.344447	-0.832254	1.175949
6	-6.123017	-1.560086	1.917886
7	-6.765898	-1.157208	3.049194
7	-6.933824	-2.514863	1.381630
6	-7.960129	-1.850686	3.216906
1	-8.611696	-1.669910	4.057648
6	-8.065431	-2.704887	2.168550
1	-8.830861	-3.418009	1.905046
6	-6.676995	-3.238503	0.157130
6	-6.990753	-2.626609	-1.070003
6	-6.156355	-4.542197	0.245137
6	-6.741738	-3.354874	-2.240747
6	-5.930115	-5.232412	-0.952916
6	-6.214062	-4.644070	-2.185033
1	-6.975289	-2.902374	-3.200782
1	-5.530232	-6.242027	-0.910776
1	-6.031886	-5.195239	-3.103736
6	-6.288575	-0.139463	3.958712
6	-6.723570	1.185614	3.774218
6	-5.432277	-0.519681	5.007249
6	-6.257252	2.152692	4.674231
6	-4.992616	0.482976	5.881675
6	-5.397715	1.806919	5.716654
1	-6.578972	3.183631	4.552981
1	-4.331018	0.214189	6.700839
1	-5.048776	2.570163	6.407046
6	-7.653372	1.571869	2.649436
1	-7.181317	1.428008	1.669790
1	-8.573266	0.975674	2.653464
1	-7.934970	2.625731	2.732469
6	-4.981775	-1.948246	5.189576
1	-5.825310	-2.648216	5.188864
1	-4.303606	-2.255828	4.384023
1	-4.447389	-2.061745	6.137374
6	-5.856954	-5.194756	1.573289
1	-5.211667	-4.568596	2.199055
1	-6.772765	-5.385987	2.146546
1	-5.354631	-6.154603	1.421216
6	-7.575092	-1.237038	-1.144927
1	-8.430585	-1.116786	-0.470178
1	-6.834263	-0.477018	-0.867074
1	-7.912093	-1.019372	-2.162822

XIVb

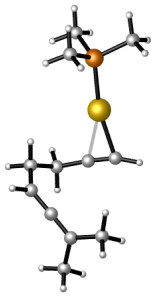


E = -2309.746015 h.
G = -2309.018446 h.

6	-0.377087	0.550430	-0.671838
6	-0.905165	1.148697	-1.974183
6	-0.191564	1.808582	0.174938
1	0.576085	0.047223	-0.834266
6	-2.194903	1.509990	-2.024640
1	-0.206771	1.305304	-2.790788
6	-1.278467	2.356490	0.736398
1	0.802185	2.240441	0.246999
6	-3.049226	1.370590	-0.841005
1	-2.639843	1.944172	-2.916443
6	-2.605304	1.779081	0.497795
1	-1.224369	3.253178	1.348582
1	-4.121793	1.393881	-1.006418
1	-3.394226	2.060029	1.188587
6	0.004796	-4.186682	0.659694
6	0.887573	-6.037387	1.630199
1	1.201867	-6.665774	2.449113
6	0.943986	-6.218071	0.286999
1	1.314614	-7.038033	-0.308570
7	0.309462	-4.789084	1.841977
7	0.401109	-5.075636	-0.292497

6	0.312460	-4.860513	-1.719158
6	1.405011	-4.266957	-2.377793
6	-0.844980	-5.281713	-2.396582
6	1.304682	-4.080313	-3.762455
6	-0.898536	-5.074713	-3.781382
6	0.162890	-4.476052	-4.458768
1	2.136055	-3.624320	-4.293546
1	-1.783139	-5.392848	-4.326470
1	0.104525	-4.325784	-5.533467
6	0.106604	-4.211805	3.151444
6	1.088100	-3.345962	3.666712
6	-1.042914	-4.574161	3.876194
6	0.879053	-2.816292	4.946974
6	-1.203851	-4.024722	5.154687
6	-0.255981	-3.149401	5.684468
1	1.623461	-2.144375	5.365871
1	-2.081113	-4.294670	5.736335
1	-0.396886	-2.734351	6.678900
6	2.327755	-2.984300	2.885228
1	2.805370	-3.865234	2.441945
1	2.094152	-2.293809	2.065112
1	3.058340	-2.493472	3.535081
6	-2.076637	-5.518026	3.311353
1	-2.549249	-5.105583	2.412055
1	-1.640637	-6.483910	3.030135
1	-2.862803	-5.706730	4.048394
6	-2.003126	-5.926738	-1.675786
1	-2.711523	-6.344959	-2.396669
1	-1.675354	-6.734397	-1.011365
1	-2.545352	-5.199350	-1.059199
6	2.646128	-3.834870	-1.635334
1	2.433359	-3.009093	-0.945385
1	3.072937	-4.650476	-1.040089
1	3.411021	-3.493584	-2.338867
6	-1.406479	-0.384522	-0.041847
6	-2.676531	0.122920	0.221147
79	-0.777611	-2.290753	0.337651
79	-4.328531	-0.824249	1.060215
6	-6.042926	-1.639168	1.876344
7	-6.659605	-1.247580	3.026796
7	-6.856644	-2.605723	1.363674
6	-7.838988	-1.957747	3.228615
1	-8.468024	-1.786424	4.088356
6	-7.962474	-2.812424	2.183236
1	-8.724911	-3.536508	1.941727
6	-6.626582	-3.330819	0.134998
6	-6.948966	-2.715799	-1.088586
6	-6.125597	-4.642816	0.215745
6	-6.723904	-3.447267	-2.262250
6	-5.924758	-5.336559	-0.984823
6	-6.214444	-4.743934	-2.213452
1	-6.963800	-2.991570	-3.219226
1	-5.540320	-6.352312	-0.947006
1	-6.051378	-5.297310	-3.134414
6	-6.177027	-0.219773	3.921888
6	-6.618583	1.102126	3.730331
6	-5.311003	-0.587212	4.966764
6	-6.149280	2.078645	4.618487
6	-4.868543	0.424267	5.829564
6	-5.280050	1.745238	5.656849
1	-6.476754	3.107071	4.491233
1	-4.199581	0.164787	6.645752
1	-4.929166	2.515530	6.338395
6	-7.557485	1.475679	2.609162
1	-7.081479	1.347829	1.629100
1	-8.464274	0.859841	2.609497
1	-7.861029	2.522930	2.698721
6	-4.853475	-2.012411	5.157375
1	-5.694575	-2.715132	5.174679
1	-4.185033	-2.325935	4.346207
1	-4.307085	-2.113730	6.099542
6	-5.821734	-5.302449	1.539539
1	-5.198103	-4.668235	2.178694
1	-6.737992	-5.523405	2.101488
1	-5.295998	-6.248756	1.381342
6	-7.519812	-1.320502	-1.158349
1	-8.361968	-1.189076	-0.469047
1	-6.765748	-0.568156	-0.895794
1	-7.872688	-1.102949	-2.170935

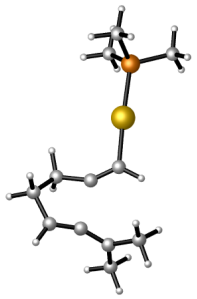
XVa



E = -946.874555 h.
G = -946.632955 h.

6	4.326828	1.866865	2.755810
79	2.858850	2.256570	0.864872
15	1.489429	1.944478	-0.987055
6	2.245061	0.899105	-2.288820
1	2.469263	-0.092510	-1.883645
1	1.555423	0.797301	-3.134102
1	3.176979	1.357460	-2.634002
6	1.053821	3.522299	-1.811164
1	0.404831	3.325498	-2.671745
1	0.531988	4.175348	-1.105073
1	1.963806	4.026222	-2.151182
6	-0.107304	1.147015	-0.572698
1	-0.646968	1.762612	0.153601
1	-0.717178	1.033776	-1.475901
1	0.073421	0.161436	-0.132406
6	4.732595	0.488791	3.045979
1	5.292261	0.097657	2.188924
1	5.436002	0.542194	3.888336
6	3.574770	-0.467828	3.386399
1	3.995231	-1.480669	3.445826
1	2.860906	-0.485229	2.551802
6	2.834615	-0.165227	4.673463
1	1.990541	-0.828415	4.878986
6	3.126573	0.778559	5.537086
6	3.404344	1.710585	6.420892
6	2.790968	3.093869	6.350391
1	2.224003	3.307442	7.266908
1	3.574775	3.860260	6.276970
1	2.116391	3.202177	5.496063
6	4.356955	1.461207	7.572678
1	4.760290	0.444635	7.559014
1	5.195866	2.169598	7.538522
1	3.846846	1.618472	8.532808
6	4.054640	3.055233	2.581205
1	3.994180	4.121820	2.697115

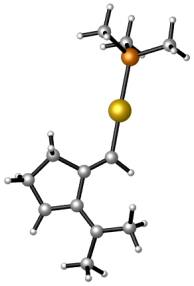
$TS_{XVa\text{-}XVIa}$



E = -946.858441 h.
G = -946.614180 h.

6	3.087633	1.013070	3.660034
79	2.161886	2.086015	1.090425
15	1.635970	2.193066	-1.188242
6	2.857498	1.351562	-2.269674
1	2.924673	0.293572	-1.997080
1	2.557421	1.433834	-3.320291
1	3.843010	1.809555	-2.138460
6	1.537451	3.908113	-1.833499
1	1.304379	3.900221	-2.904166
1	0.756931	4.458831	-1.298964
1	2.494248	4.416537	-1.677817
6	0.021810	1.432472	-1.615489
1	-0.779329	1.935753	-1.065063
1	-0.170211	1.517700	-2.690854
1	0.028168	0.374578	-1.334162
6	3.527932	-0.388710	3.441271
1	3.185598	-0.685087	2.443596
1	4.624019	-0.429834	3.448768
6	2.964950	-1.296308	4.540867
1	3.511929	-2.244270	4.588744
1	1.911016	-1.540221	4.350483
6	3.101802	-0.523870	5.826017
1	2.951931	-1.018855	6.784372
6	3.354972	0.769664	5.762389
6	3.765474	1.987830	6.165534
6	2.829078	3.152802	6.241765
1	2.881829	3.578966	7.252694
1	3.149215	3.950862	5.556080
1	1.794612	2.878384	6.027278
6	5.214571	2.250278	6.470381
1	5.816483	1.340269	6.429878
1	5.623603	2.983608	5.762288
1	5.299298	2.697147	7.469769
6	2.613766	2.093286	3.150103
1	2.417386	3.031785	3.658882

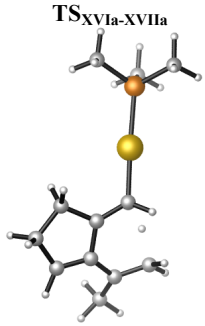
XVIa



E = -946.905015 h.
G = -946.657796 h.

6	3.035999	1.796162	3.858296
79	2.310641	1.245882	0.928379
15	1.701305	1.630944	-1.330066
6	2.384645	0.417475	-2.530823
1	2.047225	-0.590608	-2.268884
1	2.057824	0.653492	-3.549858
1	3.478780	0.437021	-2.491825
6	2.235350	3.262053	-1.991060
1	1.908077	3.389263	-3.028980
1	1.810103	4.064858	-1.379907
1	3.326911	3.335694	-1.948043
6	-0.111788	1.592650	-1.636689
1	-0.603552	2.361519	-1.031868
1	-0.331686	1.772005	-2.695048
1	-0.512898	0.616049	-1.347009
6	2.908212	3.313561	3.709197
1	3.835985	3.736323	3.301488
1	2.097849	3.589555	3.030593
6	2.692404	3.840010	5.145045
1	1.629666	4.055365	5.360300
1	3.230894	4.762324	5.395306
6	3.090062	2.716793	6.018919
1	3.206507	2.830323	7.091202
6	3.325967	1.551211	5.307137
6	3.911709	0.430055	5.941302
6	4.542080	-0.657742	5.155140
1	5.296892	-1.186044	5.744765
1	3.761592	-1.393458	4.898903
1	4.959054	-0.299458	4.209475
6	3.944974	0.253900	7.417094
1	3.391588	0.998748	7.986980
1	3.539033	-0.741633	7.649020
1	4.990596	0.227333	7.755205
6	2.822690	0.881568	2.887533
1	2.918309	-0.164592	3.182636

$TS_{XVIa\text{-}XVIIa}$

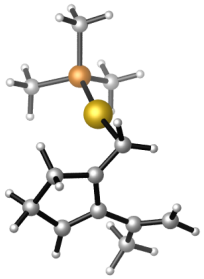


E = -946.855325 h.
G = -946.608903 h.

6	3.319474	2.157523	4.033434
79	2.851081	1.688778	1.031082
15	1.753247	1.620183	-1.061003
6	1.001735	-0.008293	-1.466138
1	0.261241	-0.271525	-0.703999
1	0.513709	0.023381	-2.446564
1	1.779089	-0.779218	-1.475349
6	2.846910	1.985409	-2.492340
1	2.280784	1.953286	-3.429984
1	3.290623	2.979220	-2.373530
1	3.654597	1.247665	-2.534575
6	0.368581	2.817279	-1.231844
1	0.747591	3.837418	-1.112208

1	-0.105470	2.722265	-2.215232
1	-0.379006	2.630827	-0.454083
6	2.127841	3.079386	4.172311
1	2.257383	3.979041	3.562869
1	1.225529	2.575384	3.800830
6	2.017384	3.380194	5.678595
1	1.010456	3.232686	6.092667
1	2.287535	4.417767	5.925455
6	2.967656	2.432979	6.307185
1	3.072357	2.335963	7.384678
6	3.695340	1.714438	5.392518
6	4.465830	0.515741	5.612144
6	5.297415	0.102358	4.564925
1	5.664886	-0.923468	4.585300
1	4.437219	0.447568	3.510468
1	6.026877	0.807312	4.165249
6	4.065791	-0.407026	6.727504
1	3.073218	-0.844450	6.550133
1	4.786486	-1.219468	6.848482
1	3.998254	0.142884	7.675520
6	3.869262	1.679489	2.846672
1	4.940381	1.802413	2.682948

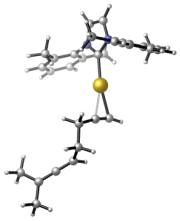
XVIIa



E = -946.948407 h.
G = -946.697091 h.

6	4.076172	2.628834	3.773213
79	3.282610	1.927929	1.377927
15	1.754094	1.402213	-0.297483
6	1.605513	-0.396699	-0.616150
1	1.268714	-0.907903	0.291022
1	0.886614	-0.578914	-1.422698
1	2.581295	-0.799820	-0.904553
6	2.192856	2.141045	-1.917010
1	1.449489	1.861597	-2.671828
1	2.227204	3.231452	-1.830000
1	3.178190	1.782847	-2.231471
6	0.049266	1.981289	0.052170
1	0.051405	3.065701	0.199850
1	-0.613122	1.730748	-0.783990
1	-0.322971	1.503528	0.963970
6	3.508029	3.992970	4.109141
1	4.279513	4.539289	4.669041
1	3.276359	4.583429	3.219545
6	2.296872	3.706800	5.018174
1	1.344978	3.833899	4.481298
1	2.247509	4.363512	5.894500
6	2.492568	2.272694	5.398423
1	1.875603	1.787740	6.148765
6	3.497680	1.656282	4.720222
6	3.892074	0.235457	4.885980
6	5.164590	-0.176525	4.759120
1	5.426704	-1.220818	4.910412
1	5.556653	1.487901	2.697894
1	5.985922	0.500740	4.548025
6	2.795880	-0.733666	5.268800
1	1.969811	-0.710933	4.546524
1	3.180748	-1.756333	5.324305
1	2.368823	-0.484198	6.248625
6	4.989797	2.412617	2.752169
1	5.437847	3.278685	2.266188

XVb

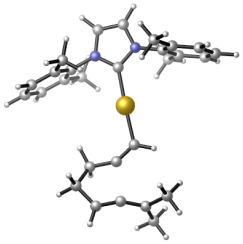


E = -1331.349534 h.
G = -1330.894795 h.

6	2.382654	2.837451	1.639272
79	1.676488	1.768821	-0.308824
6	3.729511	3.041564	3.745708
1	4.466659	2.473416	4.321399
1	2.813953	3.103325	4.347802
6	4.250854	4.433582	3.460353
1	3.538370	5.135449	3.019960
6	5.475693	4.833686	3.708513
6	6.697935	5.237170	3.968945
6	7.813643	5.115305	2.950870
1	8.233433	6.104173	2.721212
1	8.635527	4.505600	3.350295
1	7.468843	4.661903	2.017001
6	7.070127	5.852182	5.302712
1	6.214923	5.907159	5.982519
1	7.861760	5.265365	5.788323
1	7.466725	6.866936	5.161717
6	1.512039	3.501227	1.071061
1	0.800013	4.259191	0.801631
6	1.456818	0.421857	-1.817240
7	2.084036	0.421914	-3.022924
7	0.631879	-0.658034	-1.840794
6	1.656415	-0.651186	-3.793717
1	2.038252	-0.826238	-4.787605
6	0.743160	-1.329321	-3.051237
1	0.166962	-2.216112	-3.265468
6	-0.243004	-1.067748	-0.763378
6	0.213982	-2.050396	0.133751
6	-1.524252	-0.493679	-0.680834
6	-0.656266	-2.443437	1.158626
6	-2.357343	-0.920628	0.361819
6	-1.927865	-1.882547	1.275027
1	-0.328493	-3.200985	1.865296
1	-3.353462	-0.494798	0.447280
1	-2.589831	-2.203763	2.074676
6	3.060815	1.395296	-3.461298
6	4.414279	1.176422	-3.148482
6	2.617713	2.498007	-4.213933
6	5.343004	2.121196	-3.603980
6	3.585534	3.412691	-4.648947
6	4.934258	3.229105	-4.345423
1	6.395946	1.975619	-3.378411
1	5.670348	3.947636	-4.695553
6	-2.000547	0.549460	-1.662314
1	-1.499903	1.512102	-1.498378
1	-1.807175	0.257010	-2.700404
1	-3.076341	0.713324	-1.551211
6	1.159473	2.707108	-4.544447

1	0.724322	1.837486	-5.050423
1	0.562929	2.886676	-3.641460
1	1.038155	3.573565	-5.200713
6	1.586182	-2.669109	0.014608
1	1.757089	-3.097433	-0.979787
1	2.380968	-1.933092	0.188660
1	1.707190	-3.469522	0.750143
6	4.867763	-0.022688	-2.351177
1	4.537535	0.040516	-1.306629
1	4.470416	-0.959355	-2.758559
1	5.959564	-0.089721	-2.350846
6	3.423142	2.213334	2.467089
1	3.094686	1.208148	2.756275
1	4.336436	2.101447	1.871454
1	3.272086	4.272283	-5.235094

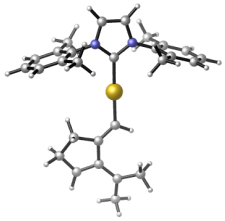
$TS_{XVb\text{-}XVIb}$



E = -1331.331858 h.
G = -1330.873841 h.

6	3.197198	3.108844	2.268326
79	2.826768	1.793880	-0.324789
6	1.612503	3.321360	4.157628
1	1.299400	2.846790	5.093988
1	0.700028	3.639307	3.635297
6	2.506654	4.504444	4.418168
1	2.231583	5.249829	5.162838
6	3.596785	4.645433	3.687859
6	4.821262	5.084931	3.337391
6	5.039595	5.918598	2.113457
1	5.556749	6.841996	2.408204
1	5.710205	5.405734	1.408492
1	4.107820	6.181619	1.609605
6	6.040638	4.685146	4.121578
1	5.788039	4.114523	5.017617
1	6.717214	4.088984	3.494533
1	6.594203	5.588220	4.411037
6	3.570837	3.196400	1.040359
1	4.232235	3.947135	0.618760
6	2.138245	0.463258	-1.725184
7	2.538363	0.341453	-3.019286
7	1.182332	-0.491319	-1.561093
6	1.841049	-0.679544	-3.657464
1	2.019018	-0.930448	-4.691736
6	0.987927	-1.202586	-2.740998
1	0.268953	-2.004282	-2.810977
6	0.455667	-0.737668	-0.335648
6	0.984163	-1.654436	0.590885
6	-0.765236	-0.068213	-0.133340
6	0.252783	-1.883972	1.763924
6	-1.459087	-0.330248	1.054872
6	-0.954853	-1.226918	1.996834
1	0.637872	-2.591050	2.493897
1	-2.405791	0.172684	1.233287
1	-1.509826	-1.421765	2.910683
6	3.548125	1.152702	-3.660941
6	4.890067	0.738133	-3.586644
6	3.143224	2.302765	-4.361929
6	5.848225	1.525812	-4.237635
6	4.137904	3.056260	-4.998935
6	5.477577	2.674441	-4.936462
1	6.891893	1.225663	-4.198023
1	6.234428	3.269590	-5.440386
6	-1.321576	0.899592	-1.149436
1	-0.662331	1.765539	-1.284368
1	-1.444405	0.432709	-2.133854
1	-2.299249	1.269631	-0.827574
6	1.697517	2.731806	-4.426891
1	1.038123	1.912322	-4.734076
1	1.341773	3.084339	-3.450541
1	1.574784	3.551530	-5.140662
6	2.292135	-2.369264	0.352902
1	2.348204	-2.799700	-0.652950
1	3.145767	-1.688018	0.460233
1	2.421347	-3.179530	1.076494
6	5.298327	-0.504471	-2.833241
1	5.130542	-0.391965	-1.754886
1	4.730189	-1.384350	-3.157205
1	6.361176	-0.712815	-2.986845
6	2.432537	2.355816	3.295230
1	1.801307	1.635182	2.763561
1	3.129711	1.791775	3.927073
1	3.850521	3.947031	-5.551281

XVIb

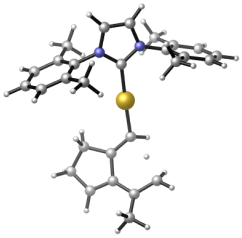


E = -1331.37814332 h.
G = -1330.917140 h.

6	3.222348	3.256960	2.324273
79	2.877608	1.717710	-0.314354
6	2.236858	2.802720	4.507210
1	2.614396	1.872827	4.971433
1	1.360369	3.088276	5.101551
6	3.323009	3.801410	4.607564
1	3.608410	4.253699	5.551676
6	3.873844	4.103564	3.371924
6	4.765669	5.193508	3.235866
6	5.008768	5.828106	1.917880
1	5.291641	6.879011	2.033195
1	5.863832	5.320372	1.440812
1	4.158207	5.720511	1.239223
6	5.512827	5.780663	4.379869
1	5.421813	5.233706	5.317135
1	6.575955	5.830893	4.102905
1	5.198973	6.824498	4.523870
6	3.677419	2.987187	1.080157
1	4.600909	3.498445	0.798929
6	2.116609	0.428306	-1.752432
7	2.509034	0.303721	-3.051187
7	1.123833	-0.493860	-1.605701
6	1.773147	-0.681151	-3.703907
1	1.940455	-0.925996	-4.741496
6	0.901484	-1.183263	-2.793904
1	0.153059	-1.956624	-2.874043
6	0.391981	-0.738126	-0.383804

6	0.906681	-1.667071	0.538292
6	-0.823075	-0.058763	-0.180261
6	0.168353	-1.899142	1.706397
6	-1.525083	-0.323601	1.002571
6	-1.034078	-1.232756	1.939434
1	0.543844	-2.615473	2.432431
1	-2.467082	0.188101	1.181373
1	-1.594885	-1.429564	2.849368
6	3.551255	1.079100	-3.684220
6	4.868666	0.587315	-3.653661
6	3.201169	2.274100	-4.338385
6	5.857933	1.340760	-4.298791
6	4.224938	2.991954	-4.970440
6	5.541296	2.532350	-4.950481
1	6.883274	0.980737	-4.290063
1	6.321455	3.100550	-5.450041
6	-1.364597	0.923706	-1.190297
1	-0.687775	1.775740	-1.326051
1	-1.501913	0.462846	-2.175735
1	-2.333151	1.312519	-0.862731
6	1.781166	2.785198	-4.359237
1	1.073976	2.021493	-4.702450
1	1.456253	3.100009	-3.359637
1	1.695973	3.649228	-5.024736
6	2.208971	-2.391660	0.299928
1	2.265304	-2.813775	-0.709546
1	3.067020	-1.717547	0.416104
1	2.328445	-3.209146	1.017224
6	5.223077	-0.699020	-2.947381
1	5.087581	-0.610083	-1.862311
1	4.599490	-1.536366	-3.281503
1	6.268630	-0.961203	-3.134107
6	1.989566	2.643798	2.990296
1	1.086572	3.202409	2.709647
1	1.835273	1.604603	2.690932
1	3.978713	3.916353	-5.486369

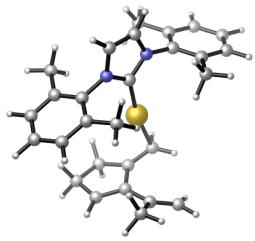
$TS_{XVIb\text{-}XVIIb}$



E = -1331.328552 h.
G = -1330.868481 h.

6	3.902003	2.868319	2.511524
79	3.171925	1.707285	-0.233615
6	3.215267	2.223980	4.750037
1	3.864334	1.576984	5.358705
1	2.239462	2.219579	5.255321
6	3.752994	3.603974	4.703799
1	3.845470	4.226514	5.589984
6	4.122998	3.995629	3.442244
6	4.372777	5.333965	2.966627
6	4.934582	5.453762	1.690401
1	4.864884	6.422728	1.195931
1	5.868800	4.935419	1.474064
1	4.244656	4.381908	1.092992
6	3.681422	6.482918	3.645218
1	3.844033	6.445017	4.730219
1	4.048153	7.442625	3.272782
1	2.593748	6.443861	3.490989
6	4.184098	2.874483	1.146705
1	5.215097	3.056446	0.839103
6	2.165363	0.606814	-1.668697
7	2.468067	0.504051	-2.993026
7	1.063255	-0.176721	-1.505772
6	1.567457	-0.330948	-3.646986
1	1.644492	-0.539020	-4.703024
6	0.683528	-0.759592	-2.711361
1	-0.169156	-1.417035	-2.783154
6	0.373113	-0.391726	-0.254091
6	0.734497	-1.501343	0.532211
6	-0.656671	0.494380	0.110294
6	0.037317	-1.701759	1.730669
6	-1.324396	0.252809	1.318308
6	-0.980755	-0.833117	2.122831
1	0.296405	-2.553363	2.354213
1	-2.125249	0.922771	1.620049
1	-1.513836	-1.008609	3.053549
6	3.576924	1.165822	-3.642334
6	4.837939	0.543436	-3.624208
6	3.343254	2.392247	-4.290885
6	5.895002	1.200115	-4.268093
6	4.431141	3.010197	-4.921160
6	5.696029	2.422888	-4.908042
1	6.878813	0.738361	-4.268651
1	6.527131	2.915637	-5.405505
6	-1.037215	1.673350	-0.752105
1	-0.246392	2.434011	-0.761297
1	-1.213840	1.379597	-1.793133
1	-1.949237	2.143513	-0.373203
6	1.976944	3.033984	-4.312009
1	1.218835	2.365805	-4.737172
1	1.641443	3.300130	-3.302258
1	1.992877	3.949358	-4.910742
6	1.837479	-2.446326	0.121296
1	1.683176	-2.844431	-0.888114
1	2.814240	-1.947512	0.124970
1	1.892866	-3.292386	0.812597
6	5.064821	-0.780746	-2.936329
1	4.988215	-0.682886	-1.846146
1	4.330463	-1.533451	-3.245257
1	6.062639	-1.164022	-3.168861
6	3.159199	1.792863	3.272986
1	2.123550	1.733905	2.912726
1	3.606345	0.809625	3.095818
1	4.276853	3.958252	-5.429521

XVIIb

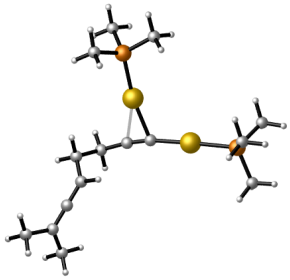


E = -1331.421594 h.
G = -1330.956436 h.

6	4.579109	2.700519	2.068110
79	3.600463	1.800818	-0.148653
6	3.688864	1.507242	3.984382
1	4.000671	1.362544	5.025512
1	2.982629	0.696074	3.755170
6	3.039573	2.838500	3.770285

1	2.243249	3.201157	4.412596
6	3.537366	3.529259	2.710457
6	3.064784	4.864733	2.271926
6	3.878203	5.765719	1.695385
1	3.504494	6.745128	1.406976
1	4.935740	5.586794	1.531974
1	5.197700	3.869086	0.364891
6	1.619136	5.200794	2.563287
1	1.430577	5.240096	3.644218
1	1.353163	6.175793	2.144083
1	0.939121	4.445056	2.150163
6	5.245728	2.909613	0.870114
1	6.119478	2.297717	0.649229
6	2.301298	0.850557	-1.402559
7	2.457049	0.687027	-2.742551
7	1.119215	0.250215	-1.103527
6	1.379353	-0.009558	-3.279306
1	1.317219	-0.238994	-4.331799
6	0.539189	-0.284343	-2.250026
1	-0.406670	-0.802502	-2.219992
6	0.534946	0.161214	0.216321
6	0.818905	-0.971128	1.000495
6	-0.322167	1.191320	0.643456
6	0.221974	-1.047353	2.266140
6	-0.891879	1.071549	1.917871
6	-0.621939	-0.035046	2.722755
1	0.420183	-1.914389	2.890530
1	-1.560545	1.851935	2.271285
1	-1.079015	-0.113978	3.705461
6	3.584510	1.159045	-3.516051
6	4.672200	0.289797	-3.716312
6	3.529609	2.452648	-4.065415
6	5.743059	0.760945	-4.486849
6	4.625164	2.878063	-4.828094
6	5.722480	2.043039	-5.035418
1	6.595283	0.109103	-4.658977
1	6.560643	2.389086	-5.634256
6	-0.636135	2.380328	-0.231868
1	0.261848	2.968013	-0.456248
1	-1.066042	2.072290	-1.192526
1	-1.355346	3.039206	0.262906
6	2.344700	3.362852	-3.850048
1	1.398567	2.869176	-4.099771
1	2.273332	3.688605	-2.804794
1	2.434015	4.258516	-4.471679
6	1.731090	-2.070238	0.511964
1	1.413848	-2.462071	-0.461277
1	2.762176	-1.714345	0.394421
1	1.743874	-2.901079	1.223031
6	4.702698	-1.100295	-3.128370
1	4.757167	-1.073213	-2.032759
1	3.807899	-1.675659	-3.392381
1	5.576294	-1.649148	-3.491817
6	4.869789	1.534883	2.994398
1	5.030772	0.596982	2.457907
1	5.801895	1.767760	3.527528
1	4.607278	3.872568	-5.265533

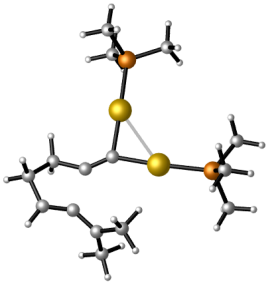
XVIIIa



E = -1543.249070 h.
G = -1542.914968 h.

6	3.095263	3.536934	2.073950
79	2.122213	2.585576	0.053984
15	1.768024	1.164245	-1.741929
6	1.298799	-0.540747	-1.257380
1	0.378647	-0.515591	-0.665243
1	1.138298	-1.155854	-2.149881
1	2.093993	-0.985078	-0.650679
6	3.222693	0.967822	-2.841478
1	2.982034	0.294283	-3.671552
1	3.517191	1.943378	-3.240832
1	4.062102	0.554776	-2.273371
6	0.413079	1.737722	-2.836866
1	0.659879	2.723813	-3.242639
1	0.267887	1.032570	-3.663054
1	-0.515480	1.816609	-2.262439
6	4.243974	2.907250	2.740666
1	5.046722	2.745789	2.011083
1	4.627904	3.623559	3.479388
6	3.919200	1.566789	3.448128
1	4.853845	1.173582	3.860462
1	3.565470	0.852619	2.691702
6	2.884365	1.701118	4.544844
1	1.886077	2.013595	4.227584
6	3.111356	1.480481	5.818160
6	3.335585	1.256513	7.092895
6	3.806996	2.354575	8.025040
1	3.093369	2.494160	8.848630
1	4.770095	2.086427	8.480632
1	3.925261	3.310053	7.505795
6	3.133324	-0.110441	7.714575
1	2.803875	-0.850401	6.979426
1	4.065440	-0.468243	8.172837
1	2.383011	-0.061984	8.515808
6	2.117927	4.174089	1.641791
79	0.572003	5.431348	1.227878
15	-1.195551	6.910414	0.818454
6	-1.444403	8.135411	2.162779
1	-0.535521	8.732435	2.288176
1	-2.283409	8.799234	1.926311
1	-1.650131	7.613230	3.102619
6	-0.999215	7.916023	-0.705270
1	-0.928444	7.256303	-1.575964
1	-1.854156	8.589577	-0.830527
1	-0.079844	8.506582	-0.640733
6	-2.823897	6.083807	0.629572
1	-3.611156	6.823189	0.445045
1	-2.787215	5.379834	-0.208077
1	-3.060692	5.526165	1.541422

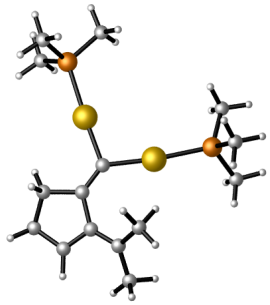
$TS_{XVIIIa\text{-}XIXa}$



E = -1543.213288 h.
G = -1542.877123 h.

6	3.365065	2.522646	3.089041
79	2.574756	3.006666	0.242318
15	2.880864	3.226418	-2.068045
6	3.355805	1.664315	-2.909603
1	2.565024	0.918651	-2.778667
1	3.513895	1.838880	-3.979840
1	4.278881	1.274663	-2.468599
6	4.204297	4.415662	-2.523607
1	4.314635	4.468977	-3.612457
1	3.955209	5.409039	-2.136874
1	5.153773	4.098092	-2.080938
6	1.400824	3.811280	-2.985874
1	1.094163	4.791706	-2.607311
1	1.617770	3.890634	-4.057125
1	0.575690	3.107210	-2.837692
6	4.867111	2.355298	2.997356
1	5.132524	2.132333	1.960954
1	5.340862	3.308749	3.265967
6	5.332760	1.270749	3.970689
1	6.382000	1.410214	4.255719
1	5.254500	0.267587	3.526386
6	4.418957	1.397824	5.154659
1	4.644228	0.893137	6.092203
6	3.307026	2.110019	5.005821
6	2.245067	2.651318	5.683464
6	2.390941	3.962203	6.398393
1	1.913515	4.759685	5.804812
1	1.865291	3.933340	7.360948
1	3.437446	4.232121	6.559493
6	2.357130	2.806571	2.345452
79	0.346984	3.246981	2.321624
15	-1.940149	3.798339	2.148639
6	-3.066455	2.355752	2.316795
1	-2.896826	1.860856	3.278530
1	-4.112754	2.675561	2.257360
1	-2.862737	1.637082	1.516410
6	-2.518924	4.982897	3.428779
1	-1.952001	5.916202	3.351460
1	-3.585675	5.198005	3.300347
1	-2.355940	4.558774	4.424933
6	-2.432538	4.574683	0.557308
1	-3.505007	4.799303	0.553205
1	-1.869807	5.502546	0.412263
1	-2.204084	3.895732	-0.270632
6	0.883484	2.130959	5.468649
1	0.505818	2.584439	4.505736
1	0.853012	1.048355	5.316927
1	0.186783	2.436159	6.255280

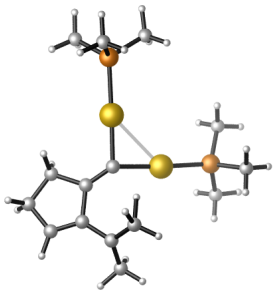
XIXa



E = -1543.230048 h.
G = -1542.892126 h.

6	3.236240	2.508484	3.104115
79	2.647247	2.876099	0.151373
15	2.962332	2.982737	-2.204512
6	3.374334	1.371045	-2.991756
1	2.557286	0.661049	-2.826294
1	3.533848	1.492465	-4.069175
1	4.283342	0.961860	-2.538656
6	4.337306	4.089487	-2.725374
1	4.457313	4.080273	-3.814599
1	4.130637	5.112810	-2.395002
1	5.271232	3.758842	-2.259045
6	1.518403	3.588049	-3.173164
1	1.254016	4.599763	-2.847925
1	1.743015	3.603365	-4.245835
1	0.658136	2.933898	-2.996840
6	4.714320	2.197842	2.796609
1	4.850728	1.117443	2.643968
1	5.053030	2.703206	1.889929
6	5.493424	2.634364	4.059051
1	5.898277	3.656504	3.948583
1	6.342679	1.998151	4.332651
6	4.456945	2.678296	5.121209
1	4.702480	2.703942	6.177842
6	3.178248	2.569871	4.610871
6	2.123115	2.281975	5.511692
6	2.086428	2.816135	6.897806
1	1.204730	3.474638	6.968469
1	1.909729	2.006730	7.617606
1	2.963476	3.399425	7.179803
6	2.283326	2.810939	2.191660
79	0.316639	3.411086	2.327322
15	-1.950046	4.130789	2.264446
6	-3.170018	2.766028	2.456177
1	-3.006624	2.253618	3.410136
1	-4.195456	3.151613	2.427659
1	-3.038221	2.039265	1.647798
6	-2.414673	5.325937	3.584258
1	-1.799664	6.227731	3.497509
1	-3.471739	5.603881	3.505295
1	-2.235398	4.878608	4.567569
6	-2.465838	4.969659	0.709579
1	-3.522172	5.258280	0.752009
1	-1.854480	5.865249	0.557166
1	-2.309775	4.296646	-0.139776
6	0.974517	1.469613	5.076835
1	0.342365	2.124741	4.436326
1	1.276454	0.652314	4.412858
1	0.375701	1.103867	5.914428

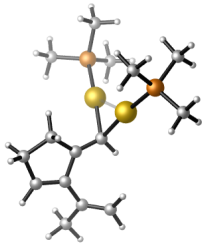
$TS_{XIXa\text{-}XXa}$



E = -1543.214220 h.
G = -1542.879590 h.

6	3.353432	2.755922	3.281696
79	2.474943	2.807268	0.366725
15	2.736843	2.764368	-1.974934
6	3.114650	1.097037	-2.650141
1	2.294978	0.410758	-2.413828
1	3.248484	1.138430	-3.736971
1	4.030781	0.713654	-2.189211
6	4.107225	3.823488	-2.587214
1	4.196361	3.749819	-3.676803
1	3.917502	4.866262	-2.312315
1	5.049763	3.510143	-2.126809
6	1.270507	3.323459	-2.932727
1	1.013877	4.349397	-2.649273
1	1.475376	3.289456	-4.008831
1	0.415768	2.676698	-2.709310
6	4.773104	3.250969	2.947455
1	5.164116	2.693607	2.090339
1	4.737459	4.304405	2.651683
6	5.638602	3.038459	4.215015
1	6.042139	3.990624	4.586502
1	6.505981	2.387830	4.038977
6	4.691752	2.430966	5.208931
1	5.007196	2.102390	6.195045
6	3.437663	2.288325	4.730994
6	2.226195	1.828444	5.370102
6	1.720251	2.538484	6.585753
1	1.466868	3.582618	6.339077
1	0.832142	2.054305	7.001601
1	2.498744	2.585747	7.357556
6	2.296521	2.735844	2.454495
79	0.267311	3.333027	2.392881
15	-1.880443	4.225062	2.241383
6	-3.227281	2.976669	2.235524
1	-3.195578	2.396146	3.163084
1	-4.203145	3.467733	2.150663
1	-3.093784	2.291932	1.392085
6	-2.300850	5.348873	3.631067
1	-1.584007	6.175288	3.665808
1	-3.311767	5.752716	3.506648
1	-2.245670	4.800830	4.577189
6	-2.179349	5.229690	0.732631
1	-3.200385	5.627455	0.732023
1	-1.467581	6.060630	0.697992
1	-2.034030	4.609804	-0.157847
6	1.400059	1.012586	4.585596
1	1.321295	1.825101	3.561163
1	1.861734	0.218657	3.993749
1	0.411443	0.757239	4.967438

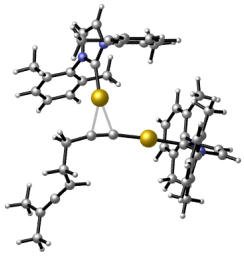
XXa



E = -1543.295099 h.
G = -1542.955024 h.

6	2.751690	2.729783	3.367014
79	2.116017	2.350610	0.405465
15	2.651071	2.247209	-1.875480
6	3.453573	0.679291	-2.396037
1	2.787713	-0.163702	-2.185078
1	3.679699	0.701334	-3.467947
1	4.382597	0.537920	-1.834403
6	3.812764	3.562893	-2.418839
1	4.028442	3.467420	-3.489042
1	3.370938	4.546218	-2.227771
1	4.747969	3.485889	-1.855159
6	1.206349	2.416759	-2.998360
1	0.705607	3.373175	-2.816468
1	1.526887	2.372507	-4.045319
1	0.494212	1.608169	-2.804969
6	3.542263	4.016492	3.176452
1	4.355832	3.822759	2.465223
1	2.930049	4.819070	2.756797
6	4.133976	4.339074	4.565315
1	3.584930	5.152850	5.063001
1	5.184103	4.653463	4.529022
6	3.951476	3.054108	5.314365
1	4.371810	2.898734	6.303641
6	3.203696	2.137048	4.646290
6	2.853727	0.793840	5.170385
6	2.684383	0.668358	6.668276
1	1.934357	1.375222	7.045463
1	2.377238	-0.344943	6.944721
1	3.620900	0.889284	7.197221
6	1.768790	2.253146	2.525894
79	0.153553	3.659576	2.151936
15	-1.714783	5.056840	2.035914
6	-3.306609	4.158377	2.214639
1	-3.335094	3.645660	3.181268
1	-4.148666	4.856671	2.150857
1	-3.397453	3.409827	1.421033
6	-1.765497	6.353253	3.336249
1	-0.893721	7.007910	3.237438
1	-2.678904	6.951349	3.244104
1	-1.738464	5.885104	4.325270
6	-1.882878	5.981308	0.457295
1	-2.788302	6.598666	0.468254
1	-1.009176	6.624800	0.312177
1	-1.938623	5.275376	-0.377465
6	2.732957	-0.277492	4.368844
1	1.337550	1.298261	2.830201
1	2.893220	-0.226158	3.296050
1	2.497025	-1.256699	4.778918

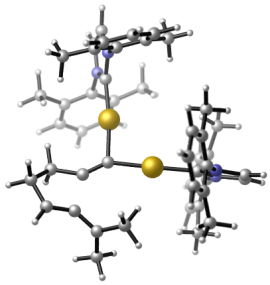
XVIIIb



E = -2312.197644 h.
G = -2311.436375 h.

6	1.948100	-0.680610	0.543789
6	2.342827	-0.612015	1.964248
1	3.433904	-0.517316	2.032393
1	1.915423	0.286938	2.424088
6	2.699561	3.032073	-1.444603
7	2.173889	4.204676	-0.999051
7	3.627119	3.389668	-2.372834
6	3.682472	4.772808	-2.504129
1	4.358627	5.252605	-3.194703
6	2.770092	5.285103	-1.639460
1	2.488594	6.303430	-1.420406
6	1.142370	4.325589	0.007108
6	-0.202912	4.312799	-0.401060
6	-1.181307	4.446229	0.593216
6	0.516745	4.606372	2.307646
6	-0.827021	4.587384	1.934380
1	-2.228963	4.442031	0.304559
1	0.790180	4.725961	3.352532
1	-1.600535	4.691025	2.690619
6	4.437861	2.471917	-3.141671
6	3.966954	2.056319	-4.400303
6	5.677336	2.063798	-2.617852
6	4.778337	1.185711	-5.139273
6	6.452147	1.192002	-3.394104
6	6.007569	0.754221	-4.641071
1	4.440341	0.853657	-6.117289
1	7.415428	0.862929	-3.013489
1	6.625276	0.082350	-5.230878
6	-0.599767	4.150578	-1.848309
1	-0.031978	4.815787	-2.508364
1	-0.428920	3.124308	-2.196821
1	-1.663529	4.370528	-1.977917
1	5.578468	2.084799	-0.455836
6	6.166051	2.530381	-1.268307
1	7.210875	2.242337	-1.119534
1	6.095016	3.618576	-1.159813
6	2.638983	2.520116	-4.948472
1	2.560053	3.613482	-4.958211
1	2.504868	2.163894	-5.974042
1	1.801650	2.141926	-4.349620
6	1.895304	-1.862772	2.765178
1	2.337735	-2.751855	2.295738
1	2.315652	-1.779398	3.772762
6	1.531224	4.478980	1.350399
6	2.983689	4.506493	1.760028
1	3.481819	3.553383	1.543489
1	3.541621	5.288719	1.231823
1	3.073843	4.696146	2.833581
6	1.539496	-0.999308	-0.590691
79	2.219349	1.153552	-0.829384
79	0.785021	-1.801758	-2.283084
6	-0.037831	-2.683754	-3.942583
6	-1.444333	-3.187047	-5.646794
1	-2.299202	-3.054885	-6.291633
6	-0.475436	-4.136642	-5.625229
1	-0.311774	-5.002662	-6.247598
7	-1.162082	-2.304015	-4.610061
7	0.378987	-3.813821	-4.576183
6	1.549661	-4.585008	-4.220462
6	2.771107	-4.283540	-4.849446
6	1.410878	-5.627823	-3.287171
6	3.887135	-5.055987	-4.501544
6	2.555798	-6.369992	-2.969749
6	3.782959	-6.087129	-3.568639
1	4.842129	-4.845156	-4.975626
1	2.474682	-7.180491	-2.250445
1	4.659068	-6.677377	-3.313564
6	-1.958082	-1.138056	-4.298466
6	-1.710163	0.050924	-5.008387
6	-2.964593	-1.247272	-3.322595
6	-2.494779	1.168417	-4.695025
6	-3.724075	-0.102896	-3.045212
6	-3.491015	1.094068	-3.721442
1	-2.323548	2.099133	-5.229461
1	-4.508765	-0.161157	-2.295656
1	-4.092832	1.970025	-3.494401
6	-0.647463	0.132850	-6.077335
1	0.337490	-0.159797	-5.696588
1	-0.873646	-0.528183	-6.923260
1	-0.571877	1.153631	-6.462997
6	-3.224457	-2.537686	-2.584399
1	-3.354475	-3.382149	-3.271121
1	-2.392490	-2.789669	-1.915127
1	-4.129479	-2.453207	-1.975834
6	0.086279	-5.947501	-2.638031
1	-0.239561	-5.138573	-1.972444
1	-0.707788	-6.095434	-3.379126
1	0.165474	-6.860814	-2.041254
6	2.897834	-3.163827	-5.854135
1	2.118586	-3.211348	-6.623121
1	2.816754	-2.182075	-5.370902
1	3.869881	-3.208061	-6.353939
6	0.391967	-2.022156	2.845020
1	-0.128047	-2.166829	1.894776
6	-0.304153	-1.994754	3.957161
6	-1.001313	-1.980589	5.070373
6	-1.577791	-0.700092	5.639938
1	-2.671380	-0.772695	5.718190
1	-1.197451	-0.522583	6.655223
1	-1.333878	0.169591	5.022790
6	-1.290361	-3.248738	5.848074
1	-0.836746	-4.127962	5.381454
1	-0.911481	-3.167949	6.876233
1	-2.373954	-3.415987	5.920525

$TS_{XVIIIb\text{-}XIXb}$



E = -2312.156130 h.
G = -2311.391948 h.

6	1.530981	-0.818742	1.440386
6	2.088513	-0.031453	2.609710
1	2.666332	0.811480	2.225284
1	1.250316	0.375396	3.190834
6	2.753783	2.834995	-1.531535
7	2.322425	4.102908	-1.278178
7	3.882591	2.998121	-2.277668
6	4.149807	4.348155	-2.486714
1	5.006212	4.677474	-3.054556
6	3.169223	5.042206	-1.858288
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6	6.362787	-0.043479	-3.816660
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1	7.292265	-0.062570	-1.872767
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1	6.820064	1.419248	-0.120098
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6	3.484670	2.155068	-5.014710
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1	3.485581	1.677302	-5.998764
1	2.481401	2.045733	-4.586746
6	2.915803	-0.956861	3.502625
1	3.946613	-1.062118	3.132775
1	2.983299	-0.574117	4.527814
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6	2.616121	4.426816	1.584761
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1	2.539783	4.717211	2.636786
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6	1.066069	-4.054070	-3.715609
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6	3.369841	-5.540497	-3.313089
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1	2.089355	-6.981093	-2.348646
1	4.274197	-6.120944	-3.151314
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6	-1.384658	0.771577	-4.899505
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1	-0.930510	-5.104693	-2.008009
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1	-0.207796	-6.722748	-1.955850
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1	3.354710	-2.132689	-5.409903
6	2.195676	-2.272528	3.451705
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1	0.210991	-3.274063	-0.019284
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1	-1.043607	-2.685934	3.688100
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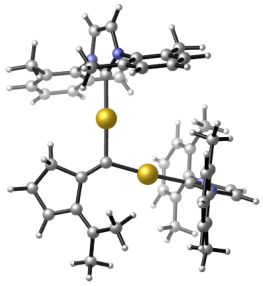
XIXb



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1	1.733344	1.216622	2.210073
6	2.871966	2.908328	-1.501431
7	2.542226	4.186013	-1.153607
7	3.892268	3.057629	-2.396021
6	4.189149	4.402955	-2.600335
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6	3.339252	5.112811	-1.819421
1	3.224050	6.175684	-1.672835
6	1.516650	4.556533	-0.206160
6	0.190665	4.681105	-0.656920

6	-0.778097	5.075616	0.275605
6	0.891348	5.211947	2.018779
6	-0.433573	5.336666	1.601261
1	-1.809791	5.181688	-0.049496
1	1.159388	5.422800	3.050722
1	-1.198059	5.646200	2.309006
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6	5.616271	1.308362	-2.374711
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6	6.316551	0.312075	-3.067888
6	6.020796	0.019491	-4.398371
1	4.786662	0.492519	-6.100709
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1	2.227252	2.383587	-4.622714
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1	1.533409	-0.055624	4.745904
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6	1.894875	4.820767	1.123277
6	3.327050	4.695147	1.584106
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1	3.994425	5.368616	1.033029
1	3.408534	4.939369	2.647426
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79	2.045781	1.163984	-0.700412
79	0.380642	-1.541717	-1.478541
6	-0.509284	-2.379982	-3.176109
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1	-2.867744	-2.643845	-5.453730
6	-0.977474	-3.704430	-4.965122
1	-0.808701	-4.502527	-5.671320
7	-1.679549	-1.996521	-3.761617
7	-0.087688	-3.438437	-3.927518
6	1.115383	-4.201403	-3.690003
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1	-1.351281	1.629520	-5.340008
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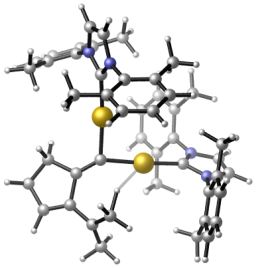

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7	3.962436	2.856621	-2.241467
6	4.256780	4.189829	-2.511270
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1	-1.923552	5.523450	1.348437
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6	0.794239	-0.323079	3.949339
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1	-0.249413	-0.106991	4.223797
6	1.321291	4.622244	0.789113
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1	2.907920	3.360946	1.550827
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6	1.340714	-0.714881	0.231772
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6	-2.259708	-2.459773	-4.641535
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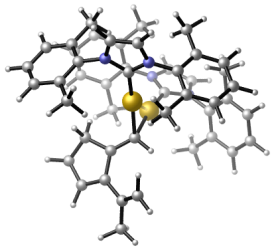

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7	4.133786	2.633384	-2.184754
6	4.478300	3.978843	-2.272682
1	5.346564	4.310561	-2.820821
6	3.543070	4.667988	-1.572581
1	3.426665	5.724052	-1.383798
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6	0.275750	4.333779	-0.927306
6	-0.827081	4.679225	-0.135125
6	0.507305	4.508980	1.874179
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1	0.594641	4.586366	2.954656
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6	0.143491	4.247961	-2.428397
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6	-1.519901	-3.256813	-5.120966
1	-1.483058	-4.027824	-5.875253
7	-1.983617	-1.583999	-3.760723
7	-0.495556	-3.084720	-4.195095
6	0.691603	-3.908311	-4.145826
6	1.810340	-3.526674	-4.908454
6	0.667557	-5.077559	-3.363830
6	2.939626	-4.354633	-4.862392
6	1.821831	-5.871106	-3.347517
6	2.948617	-5.513670	-4.087192
1	3.815214	-4.082647	-5.445757
1	1.826918	-6.780472	-2.752403
1	3.833122	-6.144677	-4.066423
6	-2.701477	-0.479985	-3.165809
6	-2.571620	0.795158	-3.745744
6	-3.533346	-0.731648	-2.060100
6	-3.299542	1.845321	-3.171644
6	-4.237043	0.351867	-1.517654
6	-4.121979	1.628531	-2.066367
1	-3.222068	2.838460	-3.605594
1	-4.888033	0.182513	-0.664098
1	-4.681998	2.455055	-1.637161
6	-1.681399	1.039479	-4.940090
1	-0.631698	0.819876	-4.710960
1	-1.961610	0.411489	-5.794161
1	-1.744739	2.084679	-5.256850
6	-3.672051	-2.110745	-1.462074
1	-3.893249	-2.866917	-2.223947
1	-2.749507	-2.422164	-0.956136
1	-4.479000	-2.126919	-0.723499
6	-0.545406	-5.476187	-2.558526
1	-0.704830	-4.795011	-1.713376
1	-1.461299	-5.464787	-3.160227
1	-0.419102	-6.484522	-2.153162
6	1.818289	-2.267333	-5.740516
1	0.925675	-2.184256	-6.370648
1	1.852846	-1.372002	-5.106929
1	2.696847	-2.246512	-6.392240
6	0.005405	-1.589055	3.314089
1	-0.096560	-2.050266	4.291815
6	1.078523	-1.750954	2.496628
6	2.269568	-2.569360	2.831471
6	3.499104	-2.271517	2.377746
1	3.698488	-1.413499	1.743444
1	4.357333	-2.877041	2.659930
1	2.344483	-1.859088	0.077452
6	2.054484	-3.743198	3.761280
1	1.707368	-3.413625	4.749394
1	1.292280	-4.429038	3.369906
1	2.983689	-4.303164	3.904931

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