Supplementary Information for

Gold(I) Complexes Bearing a PNP-Type Pincer Ligand: Photophysical Properties and Catalytic Investigations

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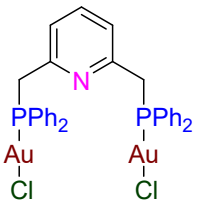
I. General methods

General Information: All air- and moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen atmosphere or in a glovebox (MBRAUN UNILAB). Solvents were purchased from commercial sources, dried by distillation under nitrogen atmosphere using the suitable drying agent and deoxygenated immediately before their use. Reagents were acquired from suppliers and used without any further purification. The DPPMPY ligand,[1] [AuCl(tht)],[2] and (Dppm)Au_2Br_2[3] were synthesized according to literature procedures. NMR spectra were recorded on the Bruker Avance 400 and 500 MHz spectrometers as solutions at 298 K and referenced to residual solvent peaks. High-Resolution Mass Spectroscopy (HRMS) experiments were carried out on a Fisons VG Quatro spectrometer.

General procedure for emission catalyst: Vinyl benzoic acid (4.90 mg, 33.07 µmol, 1 eq), $PhB(OH)_2$ (8.1 mg, 66.40 µmol, 2 eq) and Selectfluor® (17.7 mg, 50 µmol, 1.5 eq) were dissolved in CH_3CN (10 mL). After stirring for 5 minutes, the relative gold catalyst (0.992 µmol, 0.03 eq) was added and the mixture was heated at 70°C for 24 hrs. One aliquot was taken every hour during the first 8 hours and emission spectra were measured in a Horiba spectrometer with a temperature control fixed at 70°C with a λ_{ex}=350 nm. The last measure was taken after 24 hours of reaction with the same conditions as the previous experiments.

II. Synthesis of gold(I) complexes

DPPMPY$(AuCl)_2$, 1

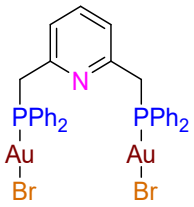


A solution of the DPPMPY ligand (404 mg, 0.85 mmol) in CH_2Cl_2 (20 mL) was added to a solution of [AuCl(tht)] (576 mg, 1.77 mmol) in CH_2Cl_2 (20 mL) at room temperature. The reaction mixture was stirred for 1 h. The insoluble colourless precipitate formed was collected by vacuum filtration, washed with CH_2Cl_2 (10 mL) and vacuum dried to afford the product as a colourless solid (560.0 mg, 70%). ^{1}H (500 MHz, CD_2Cl_2): δ 7.78 (dd, $^3J_{HP}$ = 12.9, $^3J_{HH}$ = 7.7, 8H, $CH_{Phphosphane}$), 7.51 (m, 13H, $CH_{Phphosphane}$ + CH_{py}), 7.03 (d, $^3J_{HH}$ = 7.7, 2H, CH_{py}), 4.04 (d, $^2J_{HP}$ = 12.7, 4H, CH_2P). $^{13}C\{^1H\}$ (125 MHz, CD_2Cl_2): δ 153.4 (br s), 137.6 (br s), 133.5 (d, $^2J_{CP}$ = 14 Hz), 131.8 (br s), 129.4 (s), 129.0 (d, $^2J_{CP}$ = 12

[1] Cochran, B. M.; Michael, F. E. *J. Am. Chem. Soc.* **2008**, *130*, 2786-2792.
[2] Uson, R.; Laguna, A.; Laguna, M. *Inorg. Synth.* **1989**, *26*, 85−91.
[3] Schneider, D.; Schier, A.; Schmidbaur, H. *Dalton Trans*. **2004**, 1995–2005.

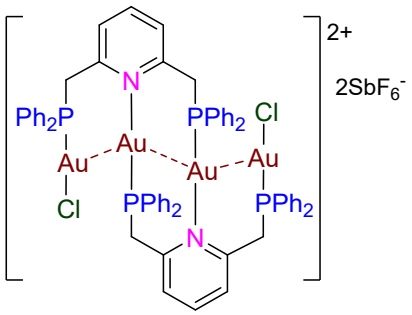
Hz), 128.9 (br s), 122.9 (t, $^{3}J_{CP}$= 4 Hz), 37.1 (d, $^{1}J_{CP}$ = 36 Hz). $^{31}P\{^{1}H\}$ (202 MHz, CD_2Cl_2): δ 33.4 (s). HRMS *m/z*: 939.133 [M+ H]$^{+}$, 904.060 [M- Cl]$^{+}$, 672.128 [M- Au – 2 Cl]$^{+}$, 1816.194 [2M- 2 Cl]$^{+}$.

DPPMPY(AuBr)$_2$, 2



A solution of KBr (131 mg, 1.1 mmol) in H_2O (15 ml) was added to a suspension of complex **1** (100 mg, 0.110 mmol) in CH_2Cl_2 (20 ml). The reaction mixture was stirred for 3 h. The aqueous phase was then separated from the organic phase and extracted three times with 5 ml portions of CH_2Cl_2. The combined organic phases were washed three times with 5 ml portions of water and dried over $MgSO_4$. The solvent was reduced under vacuum to approximately 2 ml. A colourless precipitate was formed by the addition of 50 ml of pentane. After filtration, the solid was dried under vacuum. The product was recrystallized using a mixture of dichloromethane and pentane to give a colourless solid (90.0 mg, 82 %).^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.78 (dd, $^{3}J_{HP}$ = 12.8, $^{3}J_{HH}$ = 7.9, 8H, C*H*$_{Phphosphane}$), 7.51 (m, 13H, C*H*$_{Phphosphane}$ + C*H*$_{py}$), 7.00 (d, $^{3}J_{HH}$ = 7.2, 2H, C*H*$_{py}$), 4.09 (d, $^{2}J_{HP}$ = 12.7, 4H, C*H*$_2$P). $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2): δ 153.4 (br s), 137.5 (br s), 133.5 (d, $^{2}J_{CP}$ = 14 Hz), 131.8 (br s), 129.6 (s), 129.1 (s), 129.0 (d, $^{2}J_{CP}$ = 12 Hz), 122.8 (br t, $^{3}J_{CP}$ = 4 Hz), 37.1 (d, $^{1}J_{CP}$ = 36 Hz). $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2): δ 35.1 (s). HRMS *m/z*: 1236.21 [M + Au + H], 944.09 [M – Br], 672.12 [M – 2 Br – Au].

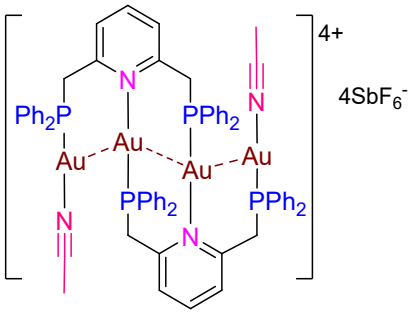
(DPPMPY$_2$Au$_4$Cl$_2$)(SbF$_6$)$_2$, 3



A solution of $AgSbF_6$ (18.2 mg, 0.053 mmol) in CH_2Cl_2 (2 mL) was added via syringe to a suspension of complex **1** (50 mg, 0.053 mmol) in CH_2Cl_2 (4 mL). The resulting mixture was stirred overnight at room temperature. The solution was filtered through Celite to give a yellowish solution. The solvent was reduced under vacuum to approximately 2 ml. Then hexane (10 ml) was added to cause the precipitation of a yellowish solid, which was filtered and dried under high vacuum (65 mg, 55 %). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.94-7.0 (br signals, 42H, C*H*$_{Phphosphane}$ + C*H*$_{py}$), 6.87(br d, 2H, C*H*$_{py}$), 6.62 (br d, 2H, C*H*$_{py}$), 4.62 (br s, 4H, C*H*$_2$P), 4.25 (br s, 4H, C*H*$_2$P). $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2): δ 156.0 (br s), 153.2 (br s), 141.6 (br s), 134.2-132.3 (br signals), 130.2-129.5 (br signals), 127.8 (br s), 127.1 (br s), 126.5 (br signal), 123.7 (br signal), 40.8 (br d, $^{1}J_{CP}$ = 35 Hz), 40.2 (br d, $^{1}J_{CP}$ = 35 Hz). $^{31}P\{^{1}H\}$

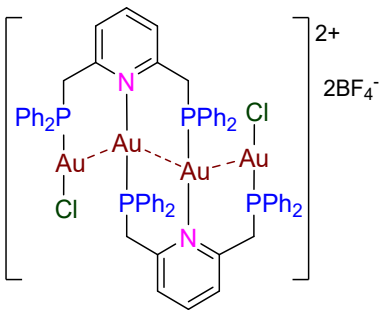
NMR (202 MHz, CD_2Cl_2): δ 35.0 (s), 28.0 (s). HR-MS (APCI-TOF) *m/z*: 1816.194 $[M + H]^+$, 1579.144 $[M- AuCl]^+$, 1396.254 $[M- 2Au – Cl]^+$, 944.038 $[M- 2 AuPhosphane]^+$.

$[DPPMPY_2Au_4(MeCN)_2](SbF_6)_4$, 4



A solution of $AgSbF_6$ (30.8 mg, 0.089 mmol) in CH_3CN (2 mL) was added via syringe to a suspension of complex **1** (42.2 mg, 0.132 mmol) in CH_2Cl_2 (4 mL). The resulting mixture was stirred overnight at room temperature. The solution was filtered through Celite to give a yello wish solution. The solvent was reduced under vacuum to approximately 2 ml. Then hexane (10 ml) was added to cause the precipitation of a yellowish solid, w hich was filtered and dried under high vacuum (150 mg, 41%). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.86-7.16 (br signals, 42H, C*H*$_{Phphosphane}$ + C*H*$_{py}$), 6.74 (br signal, 2H, C*H*$_{py}$), 6.61 (br signal, 2H, C*H*$_{py}$), 4.98-4.74 (br signal, 4H, C*H*$_2$P), 4.48-4.18 (br signal, 4H, C*H*$_2$P), 2.4 (s, 3H, C*H*$_3$, acetonitrile). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ 154.6 (br s), 154.0 (br s), 141.4 (br s), 134.2-131.9 (br signals), 130.5-130.0 (br signals), 129.9 (d, $^2J_{CP}$ = 12 Hz), 128.4 (br s), 127.1 (br s), 124.8-123.8 (br signals), 121.0 (br s), 40.1 (d, $^1J_{CP}$ = 38 Hz), 39.2 (br d, $^1J_{CP}$ = 34 Hz), 2.3 (br s) (+ acetone peaks). ^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2): δ 30.4 (br s), 25.6 (br s). HRMS *m/z*: 1073.17 [M - AuPhosphane]$^+$, 895.039 [M- Au$_2$Phosphane + Na]$^+$.

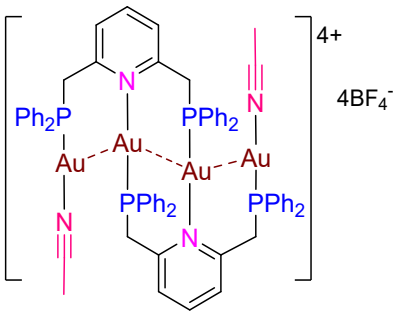
$(DPPMPY_2Au_4Cl_2)(BF_4)_2$, 5



A mixture of complex **1** (100 mg, 0.110 mmol) and $AgBF_4$ (22 mg, 0.110 mmol) in $CHCl_3$ (5 ml) was stirred overnight at 80 ºC. The volatiles were removed under high vacuum. The residue was dissolved in CH_2Cl_2 and filtered through a pad of Celite to give a yellowish solution. The solution was concentrated to 2 ml volume and then hexane (20 ml) was added to cause the precipitation of a yellowish solid, which was filtered off and dried under high vacuum (60 mg, 79%). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.09-7.25 (br signals, 40H, C*H*$_{Phphosphane}$ + C*H*$_{py}$), 7.00-6.85 (br signal, 6H, C*H*$_{py}$), 6.78 (br d, 2H, C*H*$_{py}$), 4.85-4.18 (br signals, 8H, C*H*$_2$P). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.0 (br s), 153.6 (br s), 141.5 (br s), 134.5-132.5 (br signals), 129.4-130.4 (br signals), 127.9 (br s), 127.4

(br s), 126.9 (br s), 126.3 (br s), 124.5 (br s), 124.0 (br s), 123.4 (br s), 123.0 (br s), (d, $^{2}J_{CP}$ = 12 Hz), 41.1 (d, $^{1}J_{CP}$ = 36 Hz), 40.0 (d, $^{1}J_{CP}$ = 35 Hz). $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2): δ 33.8 (br s), 29.1 (br s). HRMS *m/z*: 1816.194 $[M + H]^+$, 1796.58 $[M - Cl + Na]^+$, 1593.226 $[M – AuCl + NH_4]^+$, 944.038 [M-2 AuPhosphane]$^+$.

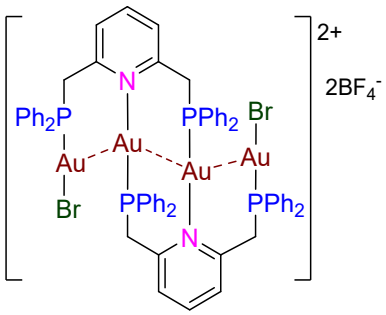
$(DPPMPY_2Au_4(MeCN)_2)(BF_4)_4$, 6



To a suspension of complex 1 (65 mg, 0.069 mmol) in CH_2Cl_2 (4 mL) was added a solution of $AgBF_4$ (26.9 mg, 0.138 mmol) in CH_3CN (2 mL) via syringe and the resulting mixture was stirred overnight at room temperature. The solution was filtered through a pad of Celite to give a yellowish solution. The volatiles were removed under high vacuum. The solution was concentrated to 2 ml volume and then hexane (10 ml) was added to cause the precipitation of a yellowish solid, which was filtered off and dried under high vacuum (100 mg, 67 %). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 7.78-7.23 (br signals, 42H, $CH_{Phphosphane}$ + CH_{py}), 6.79 (br d, $^{3}J_{HH}$ = 8 Hz, 2H, CH_{py}), 6.56 (br d, $^{3}J_{HH}$ = 8 Hz, 2H, CH_{py}), 5.26 (br dd, 2H, CH_2P), 5.13 (br dd, 2H, CH_2P), 4.35 (br t, $^{2}J_{HP}$ = 13 Hz, $^{2}J_{HH}$ = 12 Hz, 2H, CH_2P), 4.23 (br t, $^{2}J_{HP}$ = 13 Hz, $^{2}J_{HH}$ = 12 Hz, 2H, CH_2P), 2.30 (s, 3H, CH_3, acetonitrile). $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2): δ 155.4 (br s), 154.3 (br s), 141.5 (br s), 134.5-133.8 (br signals), 133.5-132-5 (br signals), 131.8 (br d, $^{2}J_{CP}$ = 12 Hz), 130.2 (br d, $^{2}J_{CP}$ = 12 Hz), 129.9 (br d, $^{2}J_{CP}$ = 12 Hz), 128.1 (br s), 127.2 (br s), 126.7 (br s), 126.5 (br s), 125.1 (br s), 124.6 (br s), 124.3 (br s), 123.7 (br s), 120.6 (br s), 40.0 (d, $^{1}J_{CP}$ = 40 Hz), 38.6 (br d, $^{1}J_{CP}$ = 33 Hz), 2.5 (br s). Datos $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2): δ 30.9 (br s), 26.0 (br s). HR-MS (APCI-TOF) *m/z*: 1816.193 $[M + Na + NH_4]^+$, 1564.206 $[M – Au + Na]^+$, 1186.221 $[M – 3\ Au + Na + NH_4]^+$, 895.095 $[M – 2AuPhosphane + Na]^+$.

0

$(DPPMPY_2Au_4Br_2)(BF_4)_2$, 7



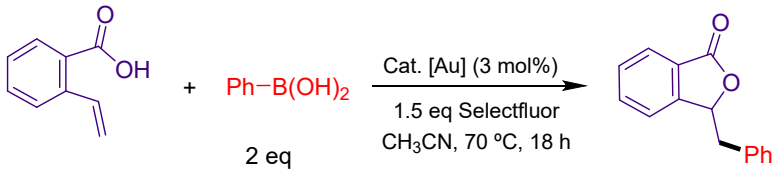
A solution of $AgBF_4$ (18.9 mg, 0.097 mmol) in CH_3CN (2 ml) was added to a suspension of complex **2** (100 mg,0.097 mmol) in CH_2Cl_2 (4 ml) and the mixture was stirred overnight. The residue was filtered through a pad of Celite to give a yellowish solution. The solution was concentrated to 2 ml

volume and then hexane (20 ml) was added to cause the precipitation of a yellowish solid, which was filtered off and dried under high vacuum (207 mg, 48%). ^{1}H NMR (500 MHz, CD_2Cl_2): δ 8.0-7.30 (br signals, 38H, $CH_{Phphosphane}$ + CH_{py}), 6.99 (br signal, 4H, CH_{py}), 6.90 (br d, 2H, CH_{py}), 6.75 (br d, 2H, CH_{py}), 4.87-4.53 (br signals, 4H, CH_2P), 4.43-4.21 (br signal, 4H, CH_2P) (+signals corresponding to acetonitrile and hexane). $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2): δ 156.2 (br s), 153.2 (br s), 141.4 (br s), 133.7-132.3 (br signals), 130.5-129.4 (br signals, CH_{Ph}), 129.3 (br s), 127.9 (br s), 127.1 (br s), 126.5 (br s), 40.9 (br d, $^{1}J_{CP}$ = 34 Hz) , 40.5 (br d, $^{1}J_{CP}$ = 35 Hz) (+signals corresponding to acetonitrile and hexane). Datos $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2): δ 34.9 (br s), 30.2 (br s). HR-MS (APCI-TOF) m/z: 1816.195 $[M - Br]^+$, 672.127 (Z=2) $[M - 2Au - 2Br]^{2+}$, 1279.21 $[M - 3Au- Br + 2Na]^+$, 944.09 $[PNPAu_2Br]^+$.

III. General procedure for catalyst screening

Vinyl benzoic acid (10.0 mg, 67.5 µmol) was dissolved in CH_3CN (1.3 mL) with $PhB(OH)_2$ (16.46 mg, 145 µmol) and the relative gold catalyst (3.3 µmol, see table below). After stirring for 5 minutes, Selectfluor® (35.86 mg, 101 µmol) was added and the mixture was heated at 70°C. After 18 hours, the solution was cooled at room temperature. The volatiles were removed under high vacuum and the solution filtered through neutral alumina. The residue was dried under high vacuum. Then 16.5 mg (67.5 µmol) of triphenylmethane were added. The reaction was monitored by ^{1}H NMR for product formation versus the peak at 5.73 ppm (relative to methinic *CH* of the lactone) and 5.59 ppm (relative to the benzylic *CH* of the internal standard).

Table S1. Catalyst screening.



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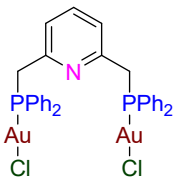
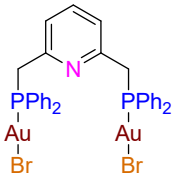
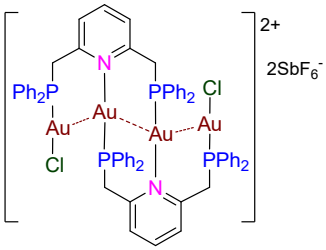
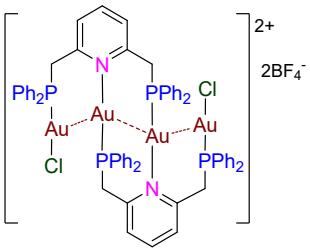
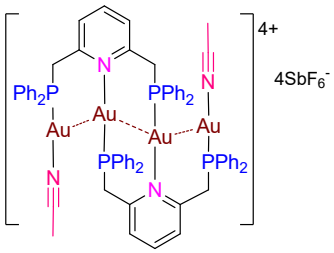
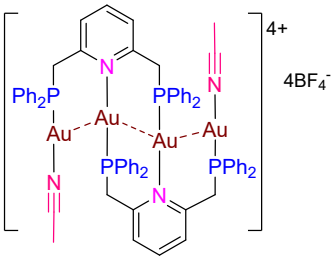
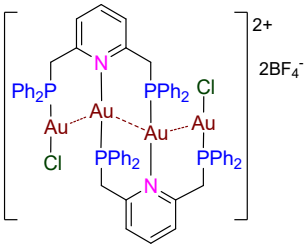
2		50
3		52

4		55
5		61
6		54
7		60
8		61
9	$Dppm(AuCl)_2$	51
10	$Dppm(AuBr)_2$	63

[a]Yields were determined via ^1H NMR analysis versus triphenylmethane as an internal standard.

IV. Absorption and Emission spectra

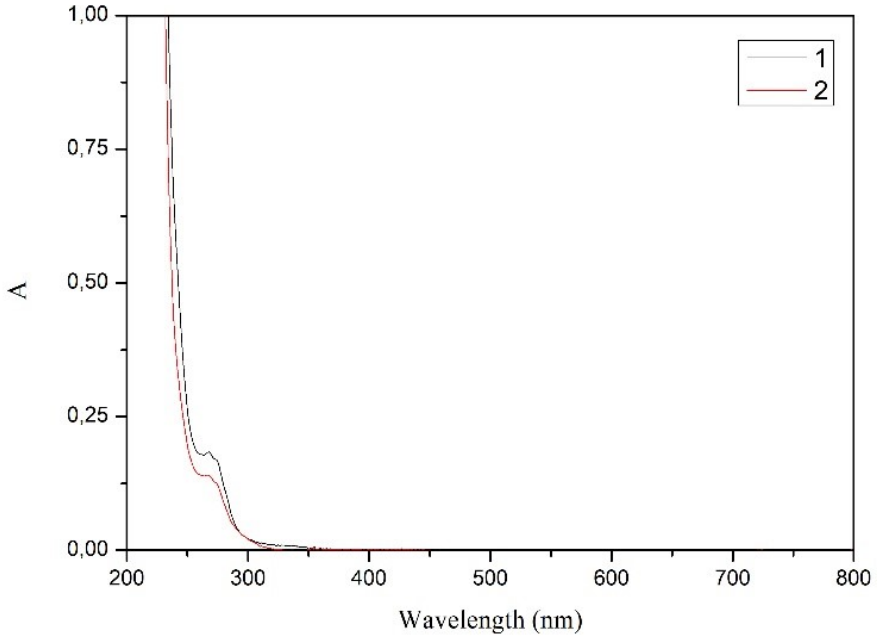


Figure S1. Absorption spectra of $1 \cdot 10^{-5}$ M dichloromethane solutions of dinuclear compounds **1** and **2**.

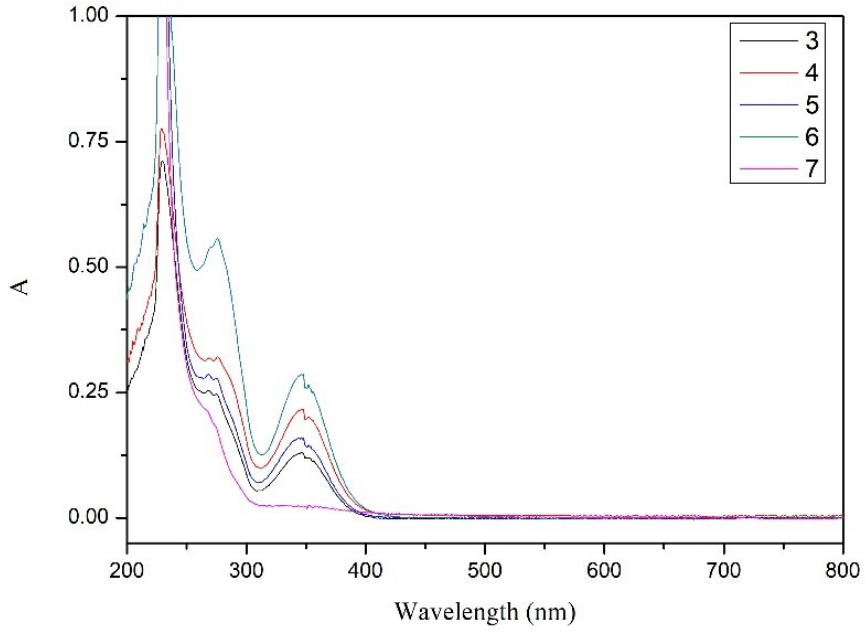


Figure S2. Absorption spectra of $1 \cdot 10^{-5}$ M dichloromethane solutions of tetranuclear compounds **3-7**.

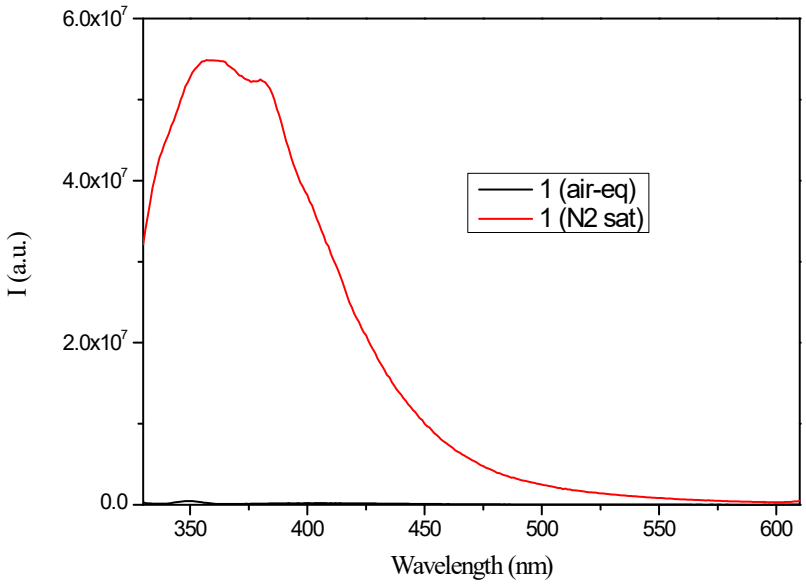


Figure S3. Emission spectra of compound **1** in $1 \cdot 10^{-5}$ M dichloromethane solutions in air-equilibrated and N_2-saturated samples. λ_{exc} = 320 nm.

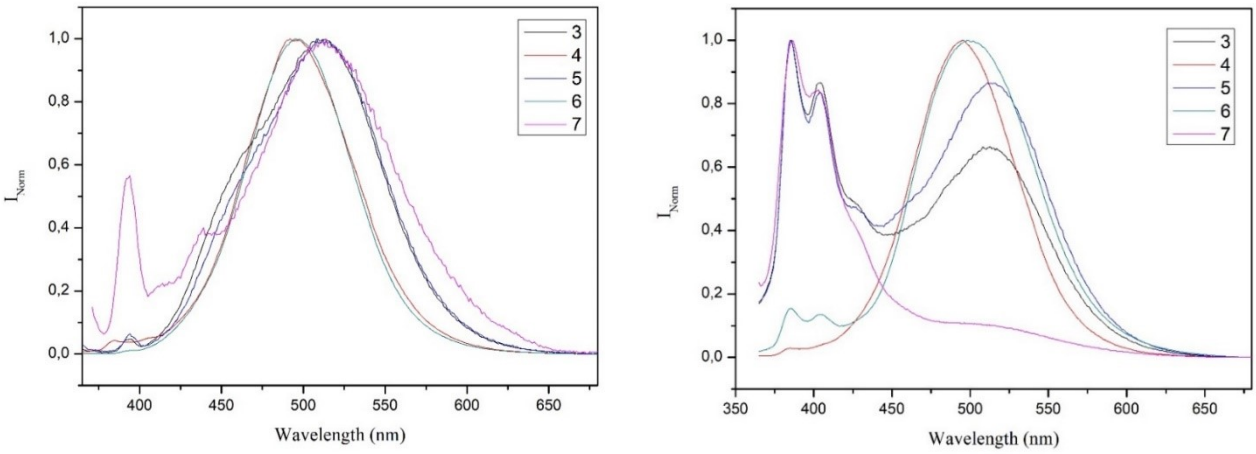


Figure S4. Normalized emission spectra of compounds **3-7** in $1 \cdot 10^{-5}$ M dichloromethane solutions in air-equilibrated (left) and N_2-saturated (right) samples. λ_{exc} = 350 nm.

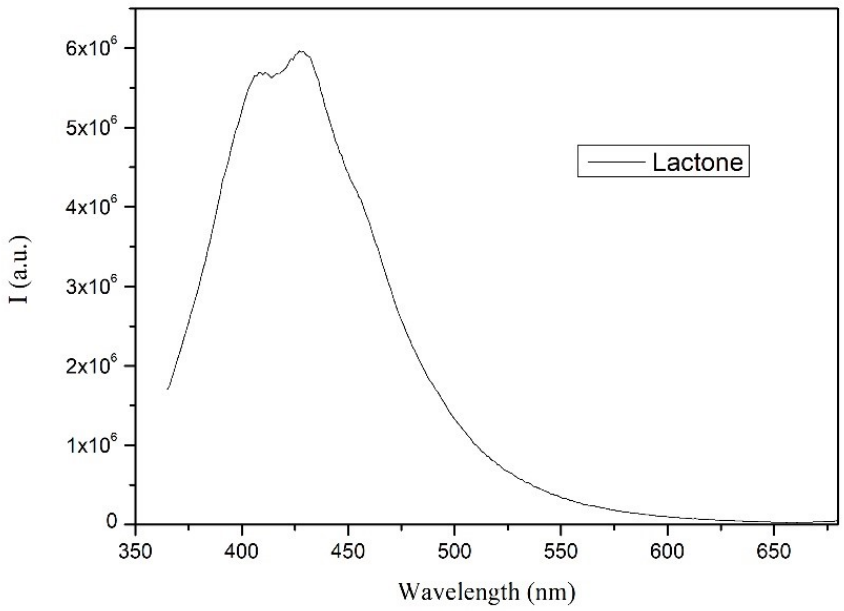


Figure S5. Emission spectra of compounds lactone 10^{-5} M in acetonitrile at 70 ºC λ_{exc} = 350 nm.

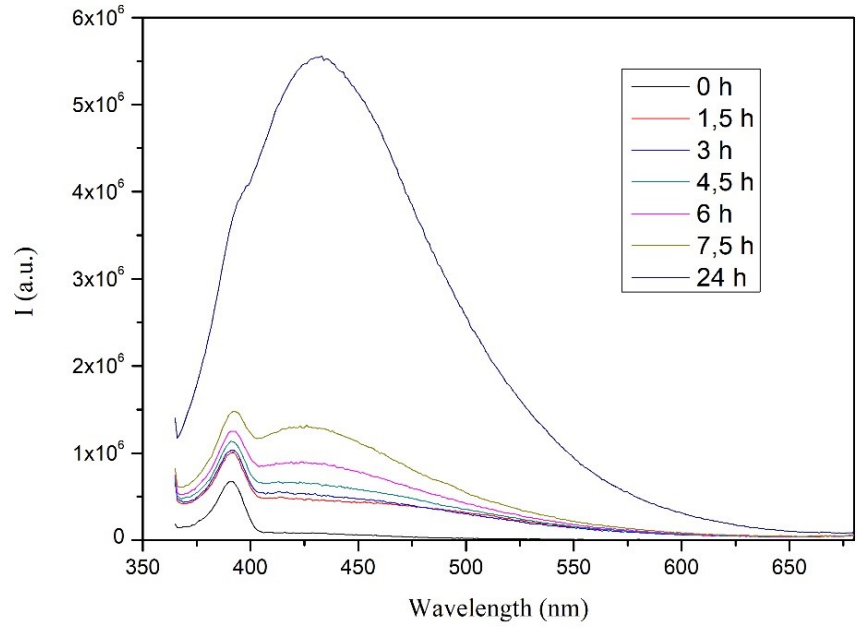


Figure S6. Emission spectra of the reaction of the catalytic reaction using **1** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 1 (3%)

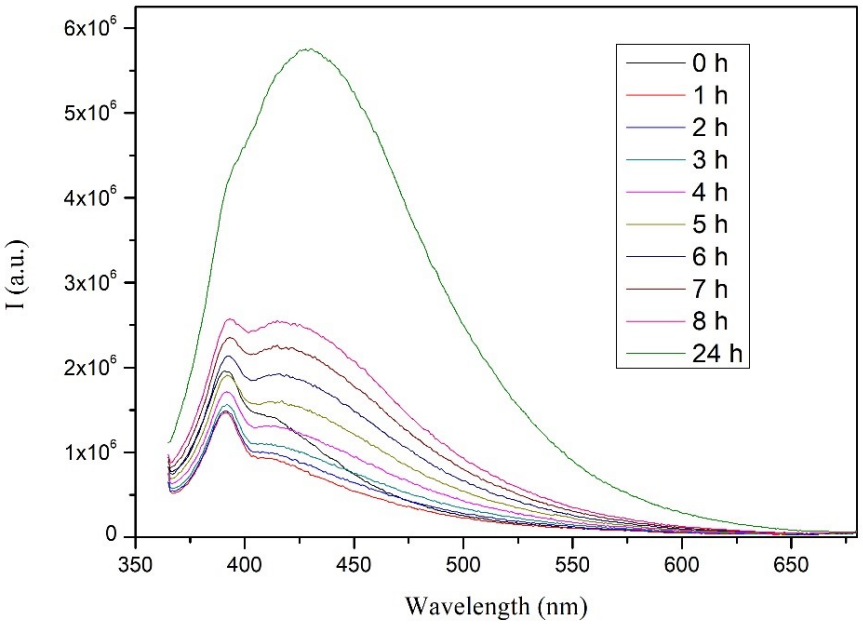


Figure S7. Emission spectra of the reaction of the catalytic reaction using **2** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 2 (3%)

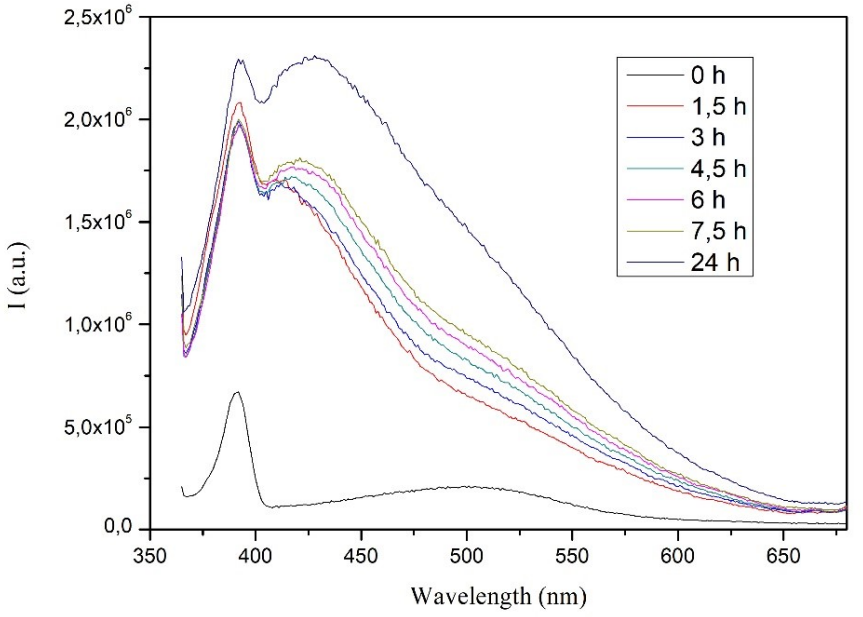


Figure S8. Emission spectra of the reaction of the catalytic reaction using **4** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 4 (3%)

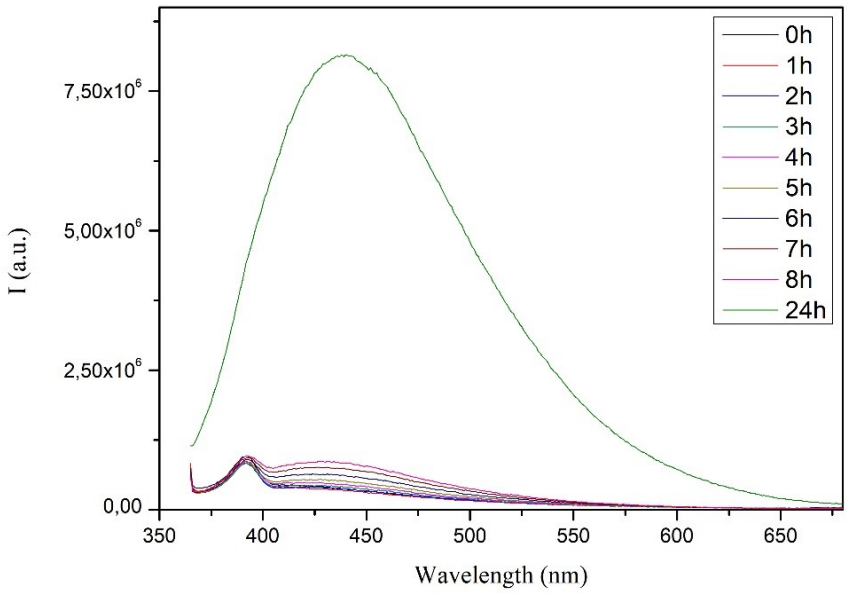


Figure S9. Emission spectra of the reaction of the catalytic reaction using **5** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 5 (3%)

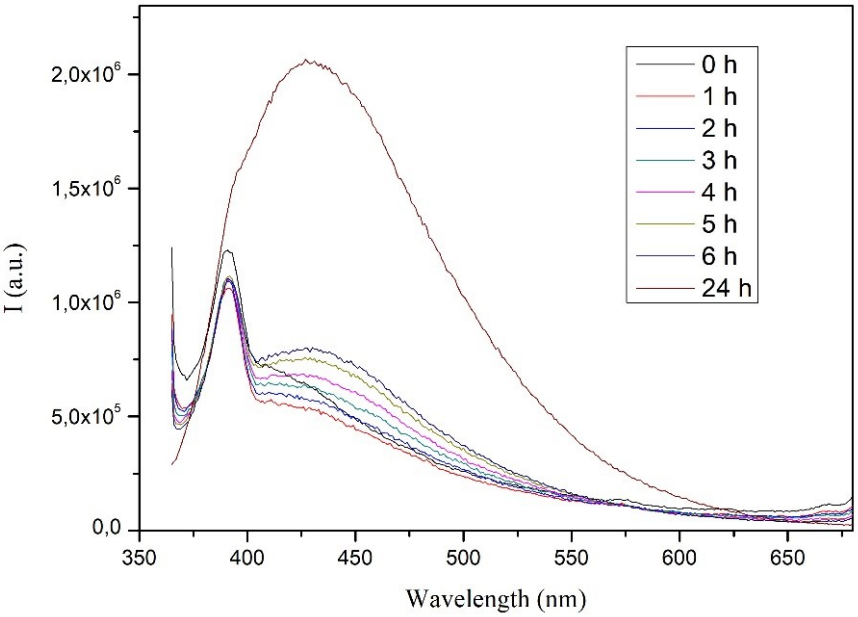


Figure S10. Emission spectra of the reaction of the catalytic reaction using **6** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 6 (3%)

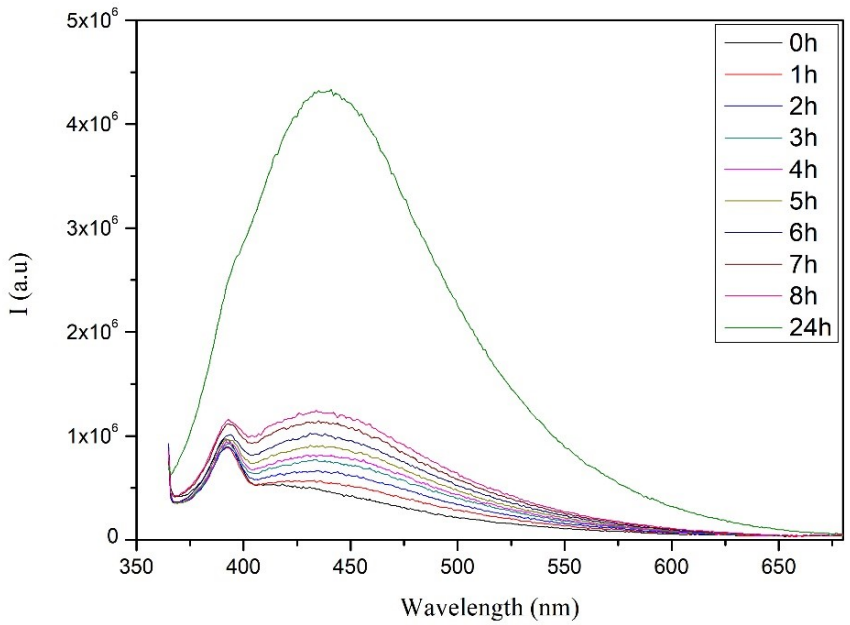


Figure S11. Emission spectra of the reaction of the catalytic reaction using **7** as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and 6 (3%)

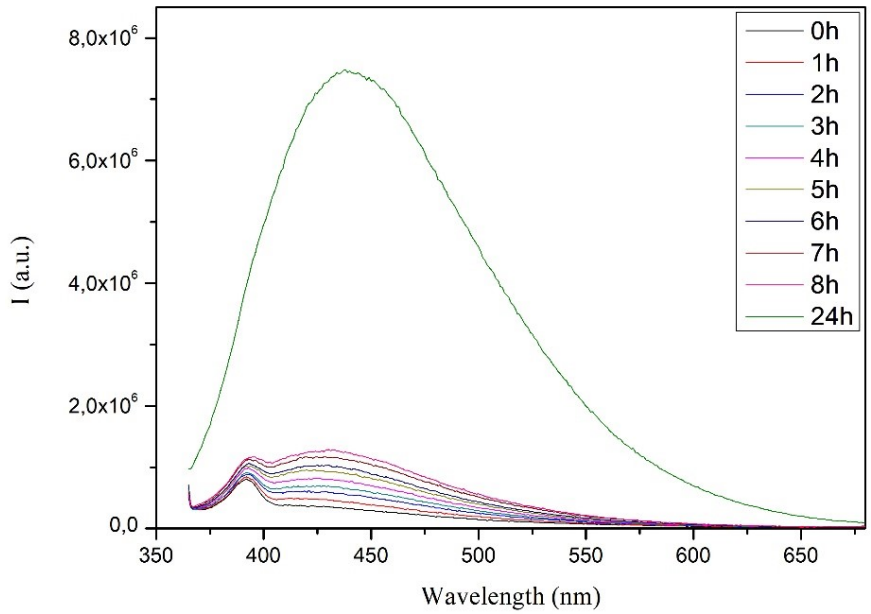


Figure S12. Emission spectra of the reaction of the catalytic reaction using dppm$(AuCl)_2$ as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and dppm$(AuCl)_2$ (3%)

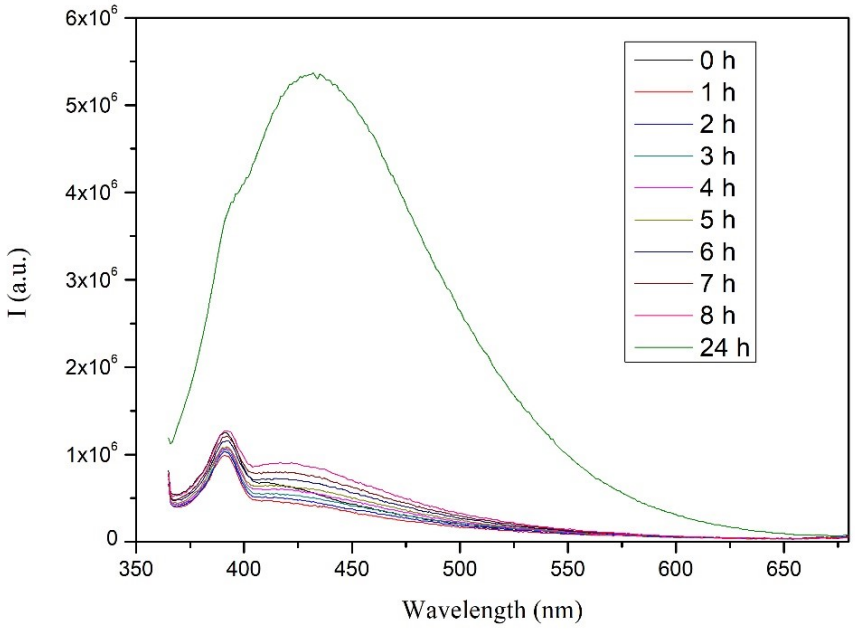
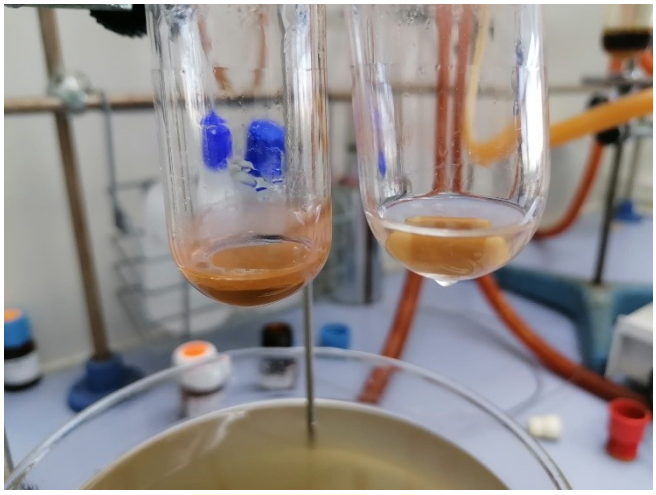


Figure S13. Emission spectra of the reaction of the catalytic reaction using dppm$(AuBr)_2$ as catalyst at different times. Experimental conditions: 70 ºC, acetonitrile, SelectF (1.5 eq) and dppm$(AuBr)_2$ (3%)

V. Mercury test for Gold Nanoparticles

Catalytic reaction



To the left – Reaction mixture of complex **7** in the absence of mercury.; To the right– Reaction mixture of complex **7** in the presence of mercury.

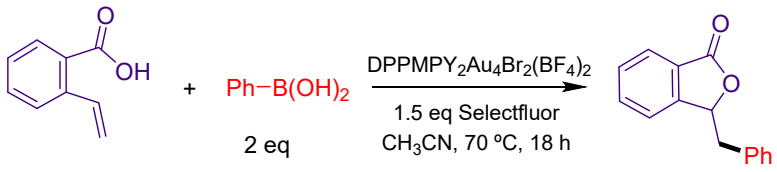
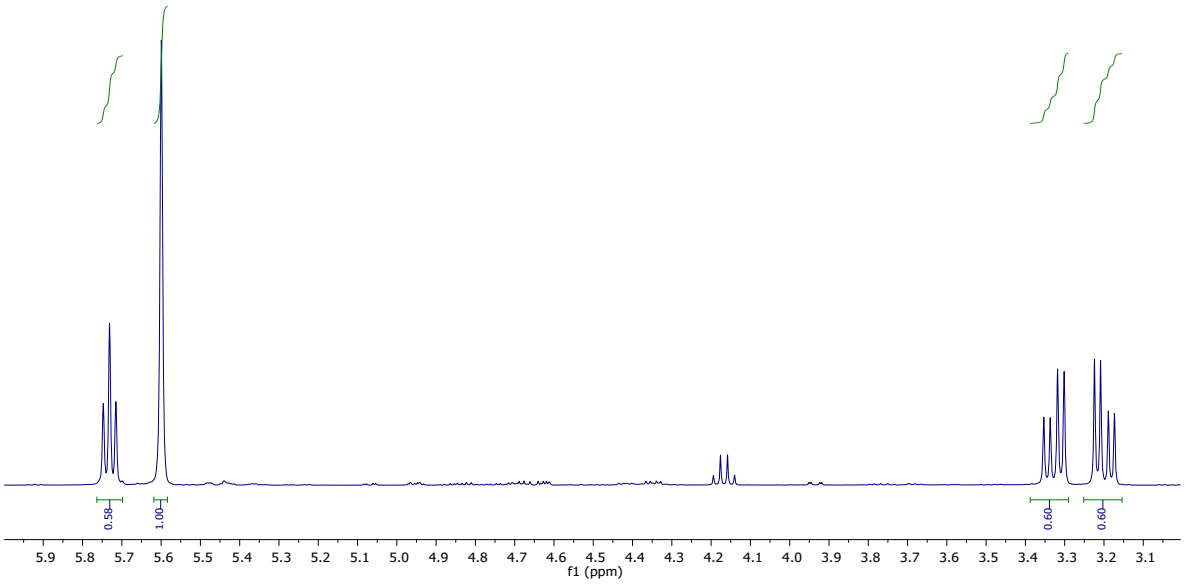
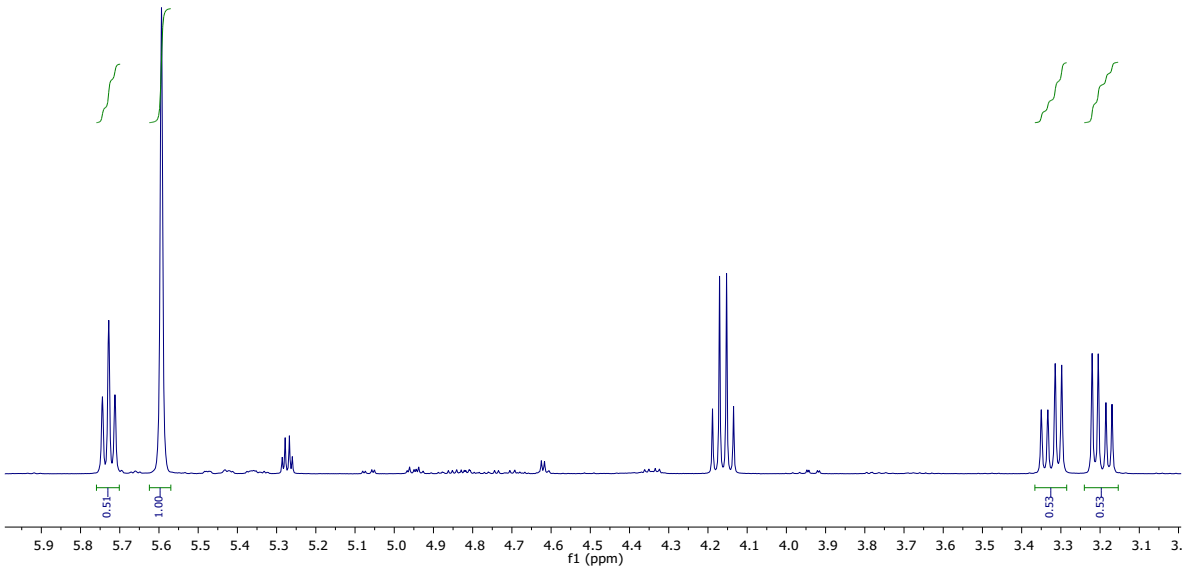


Table S2. Mercury test.

	Yield %	
	With Mercury	Without Mercury
$DPPMPyAu_4Br_2(BF_4)_2$	53	60



Without mercury.



With Mercury.

Figure S14. ^{1}H NMR spectra of the reaction mixtures

VI. ^{31}P NMR studies

In two different NMR tubes, Gold catalyst **1** and **7** (1 eq) were dissolved in 0.6 ml of CD_3CN with Selectfluor (10 eq). After one hour at room temperature the mixtures were analized by $^{31}P\{^{1}H\}$ NMR.

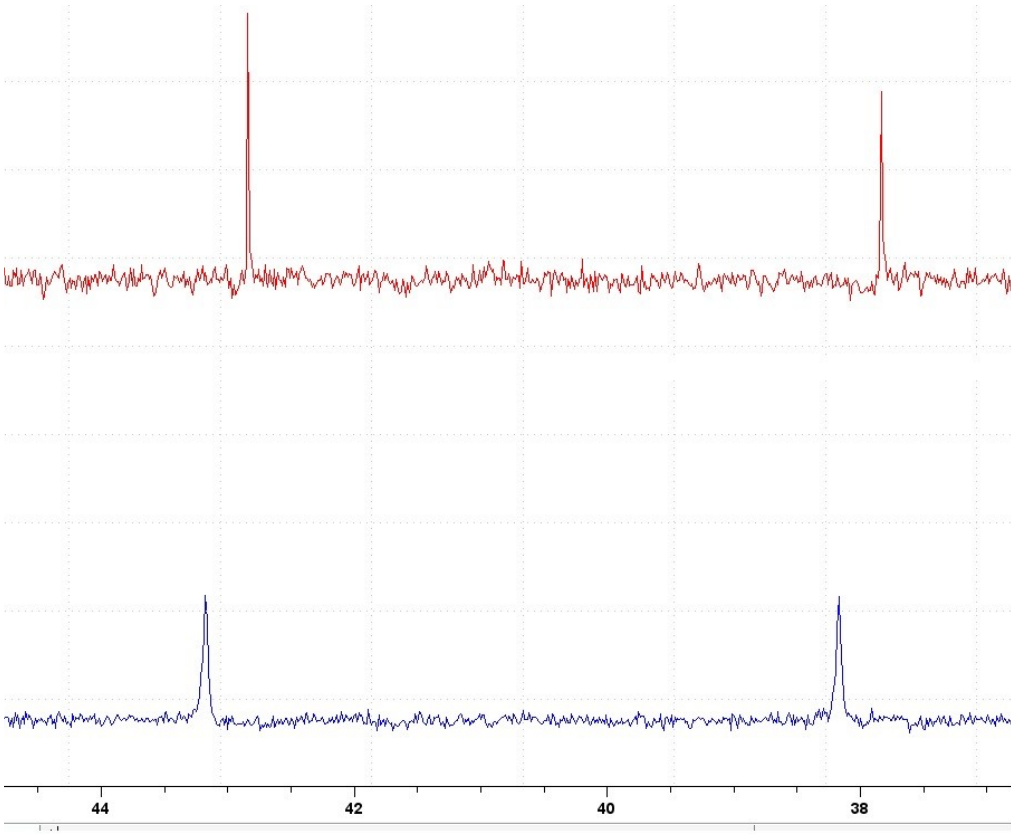
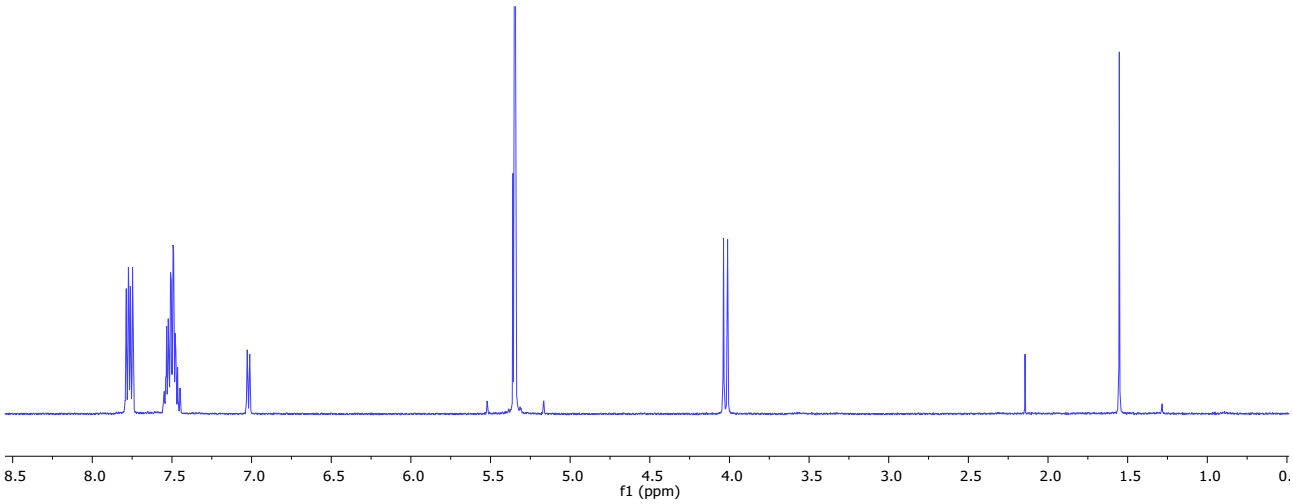


Figure S15. $^{31}P\{^{1}H\}$ NMR spectra of the reaction mixtures

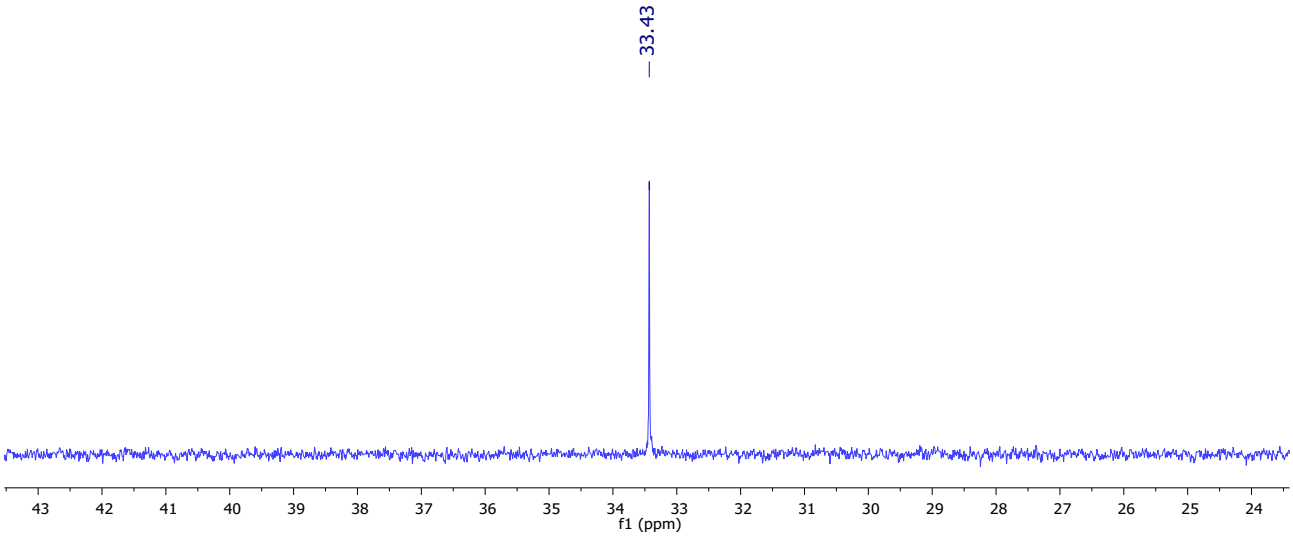
In both cases two peaks with ratio 1:1 were detected. The chemical shift moved to higher frequencies compared to those observed for complexes **1** and **7**. (Section VII)

VII. NMR spectra

^{1}H NMR



^{31}P{^{1}H} NMR



^{13}C{^{1}H} NMR

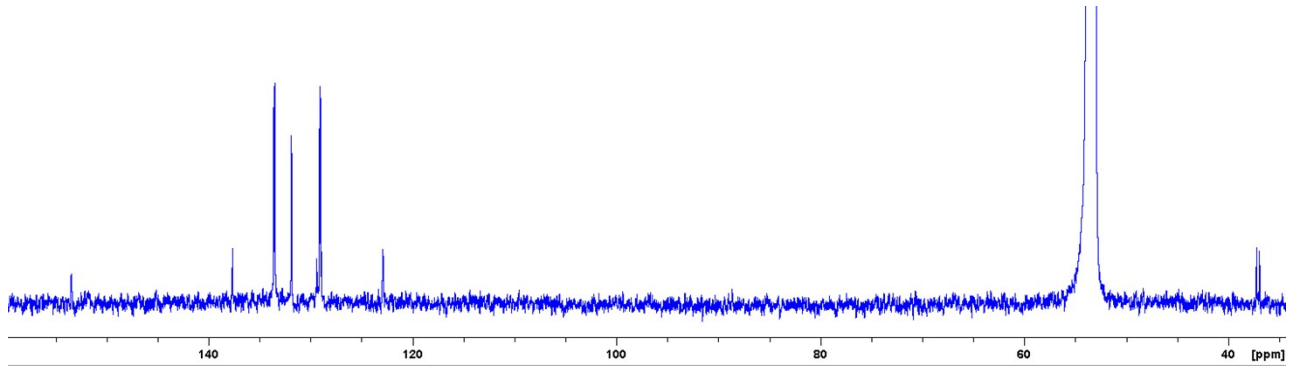
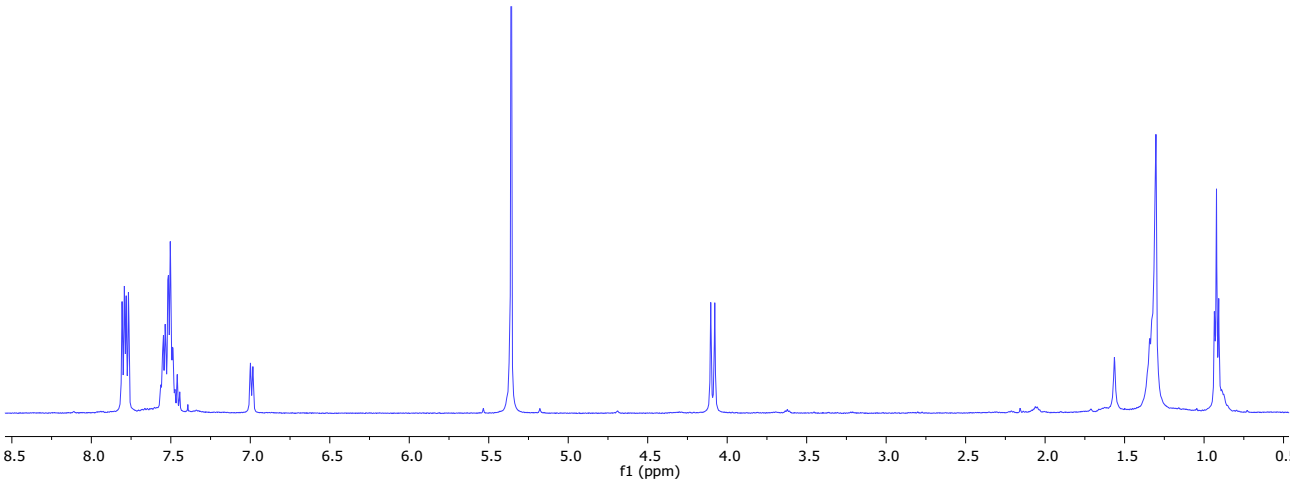
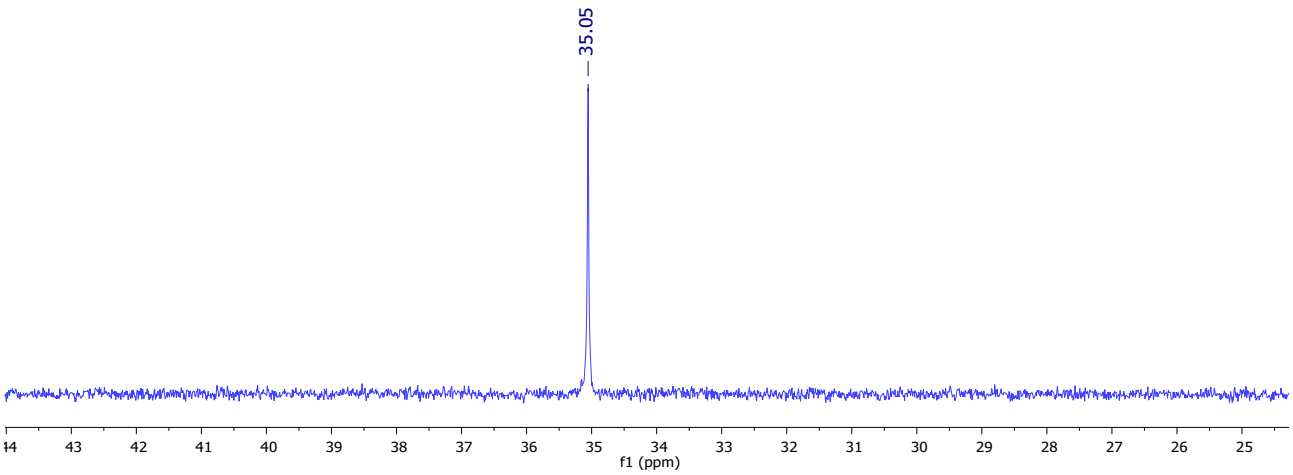


Figure S16. NMR spectra of DPPMPY(AuCl)$_2$, **1**

^{1}H NMR



^{31}P{^{1}H} NMR



^{13}C{^{1}H} NMR

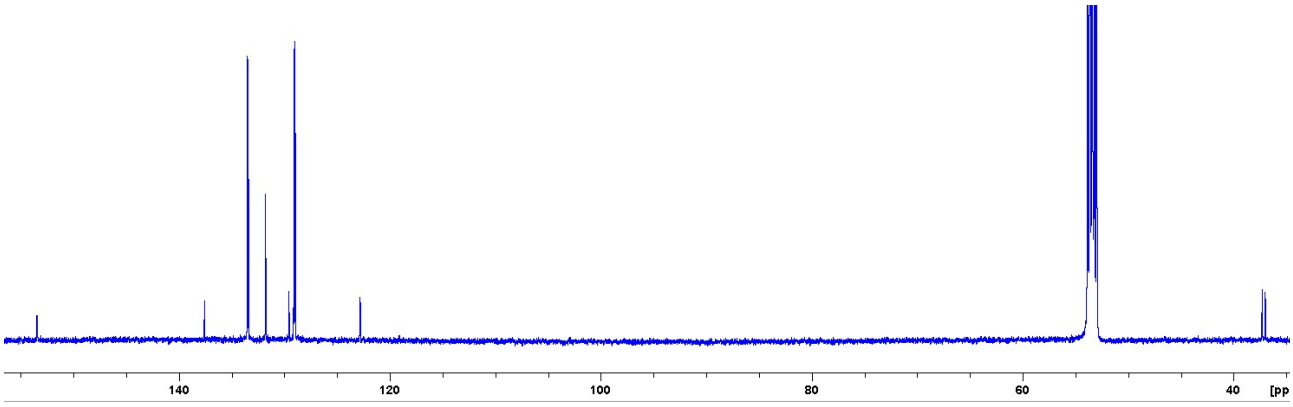
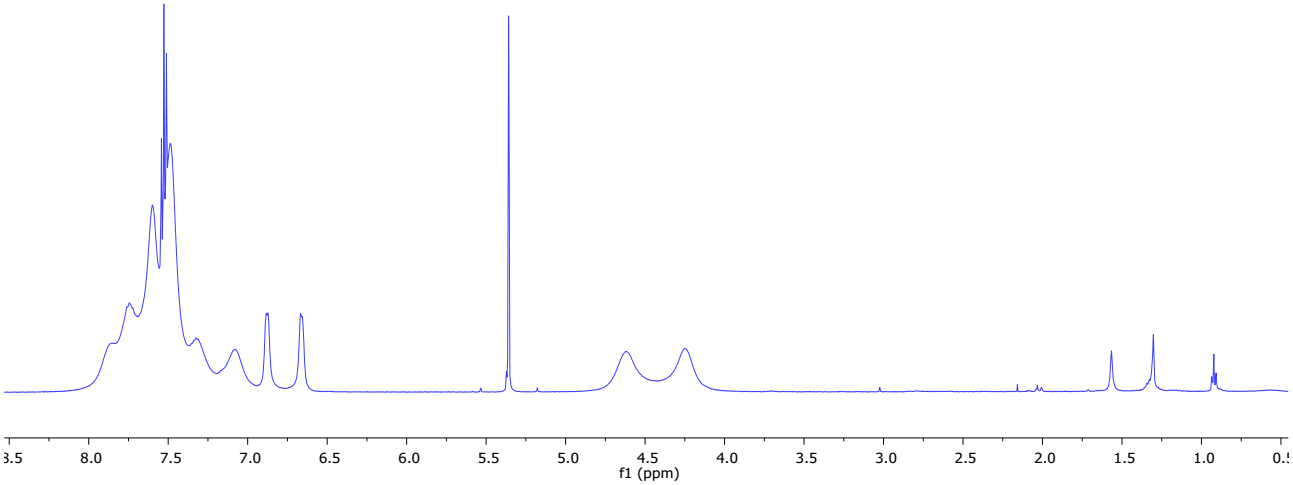
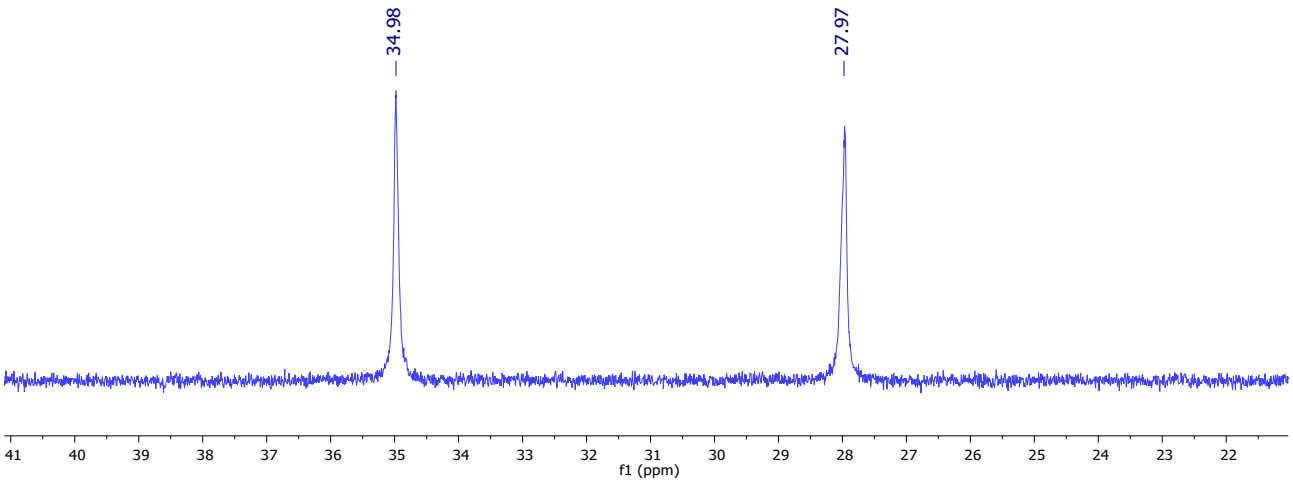


Figure S17. NMR spectra of DPPMPY(AuBr)$_2$, **2**

^{1}H NMR



^{31}P{^{1}H} NMR



^{13}C{^{1}H} NMR

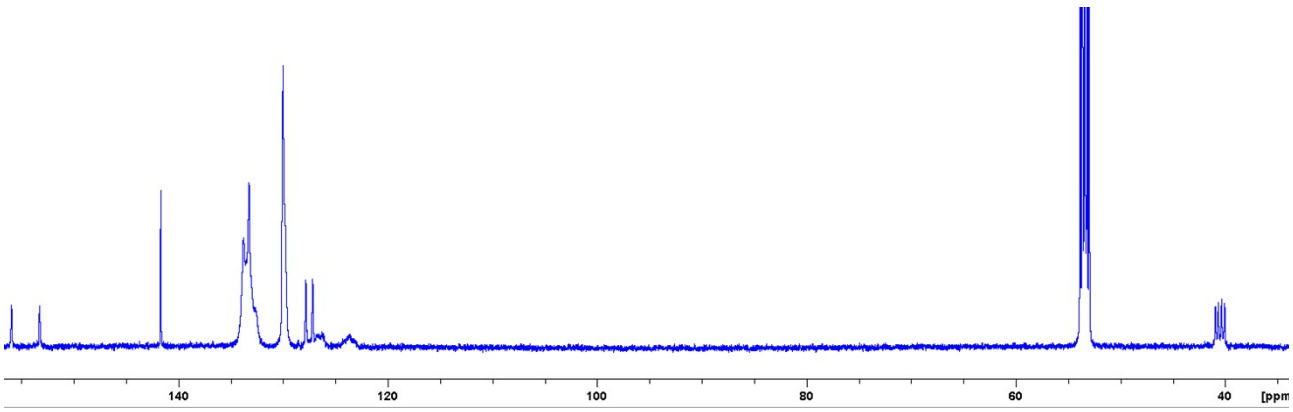
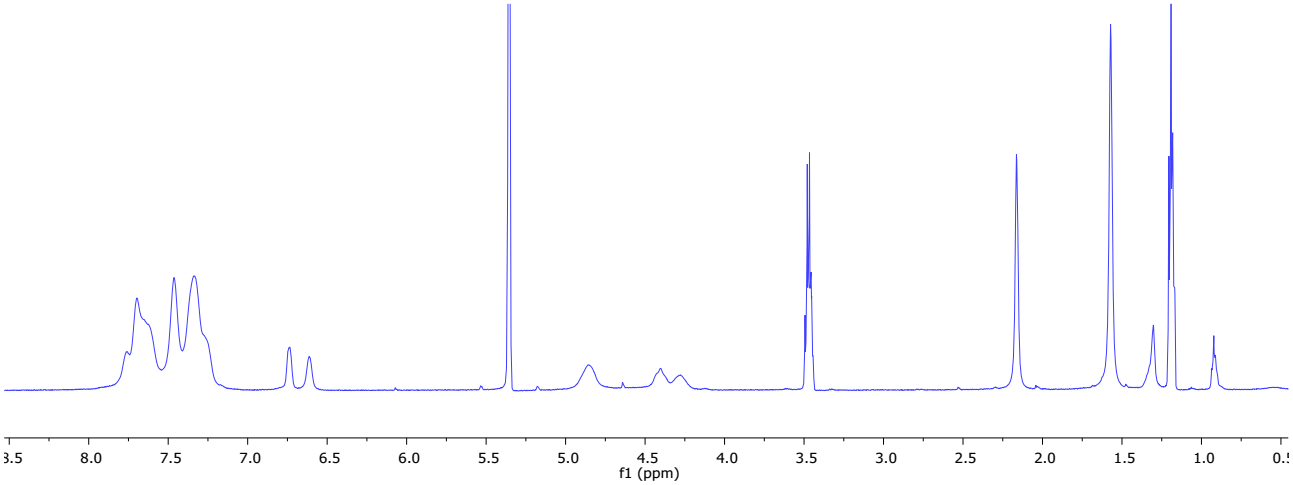
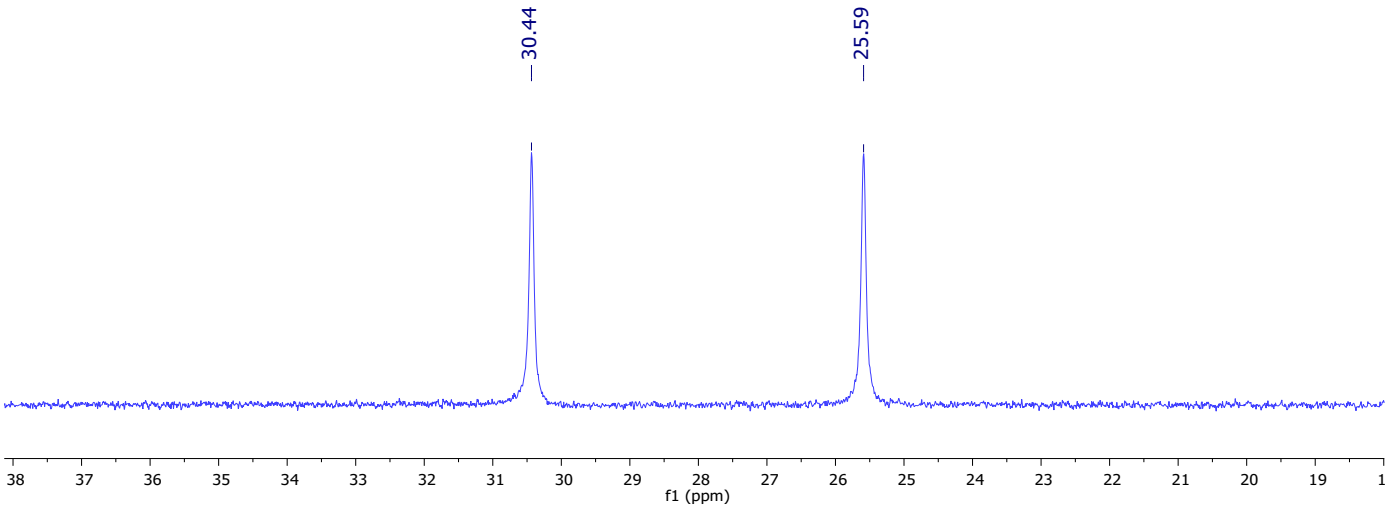


Figure S18. NMR spectra of $(DPPMPY_2Au_4Cl_2)(SbF_6)_2$, **3**

^{1}H NMR



^{31}P{^{1}H} NMR



^{13}C{^{1}H} NMR

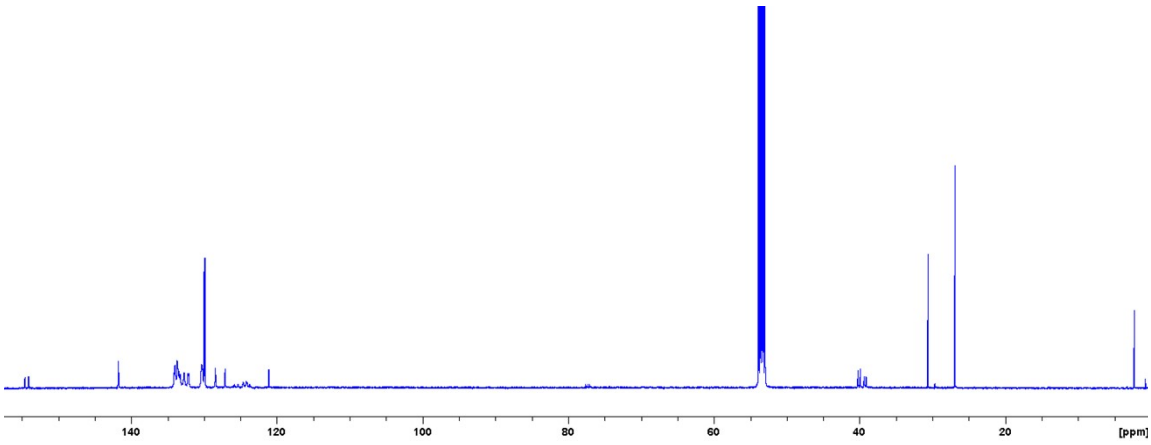
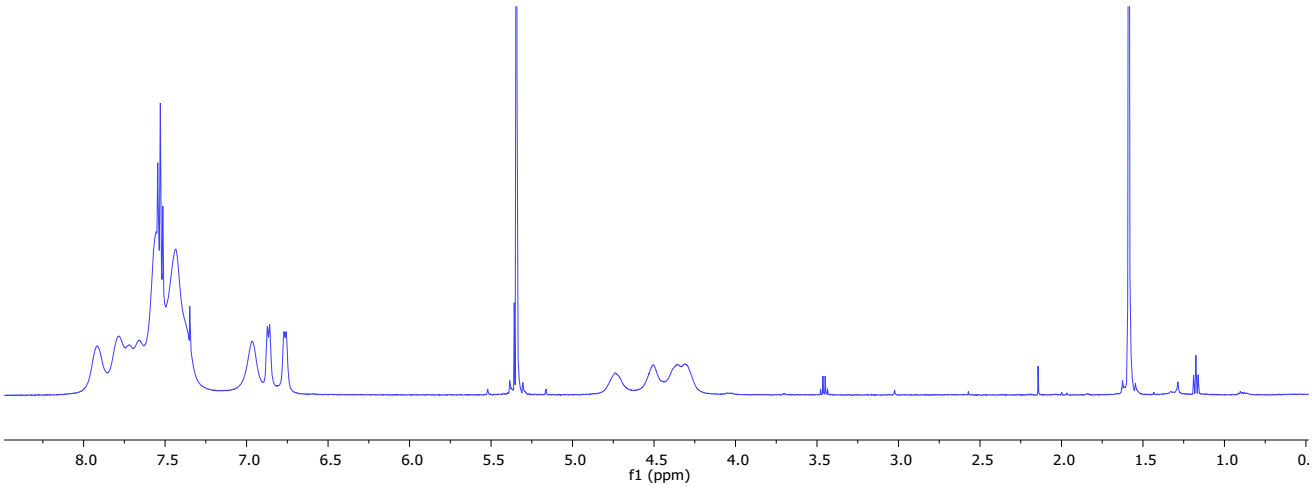
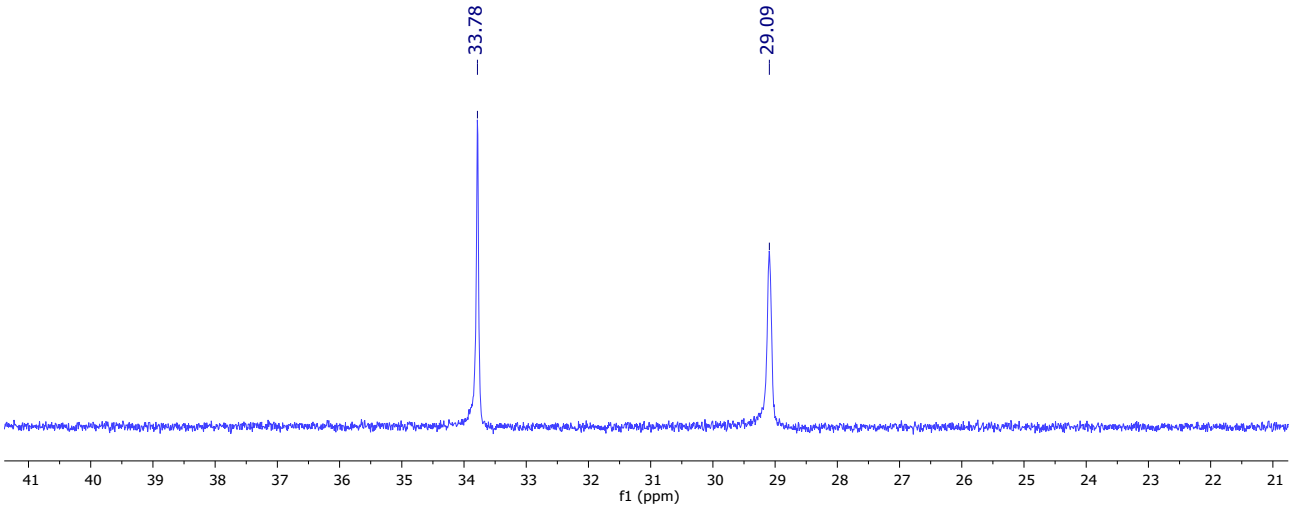


Figure S19. NMR spectra of $(DPPMPY_2Au_4(MeCN)_2)(SbF_6)_4$, **4**

^{1}H NMR



^{31}P{1H} NMR



^{13}C{^{1}H} NMR

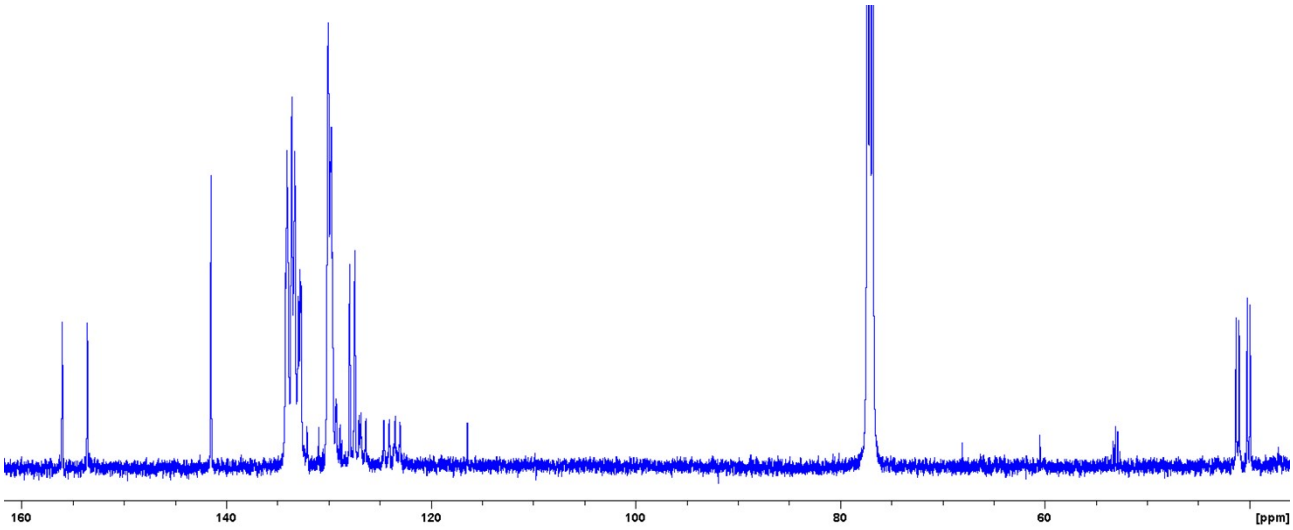
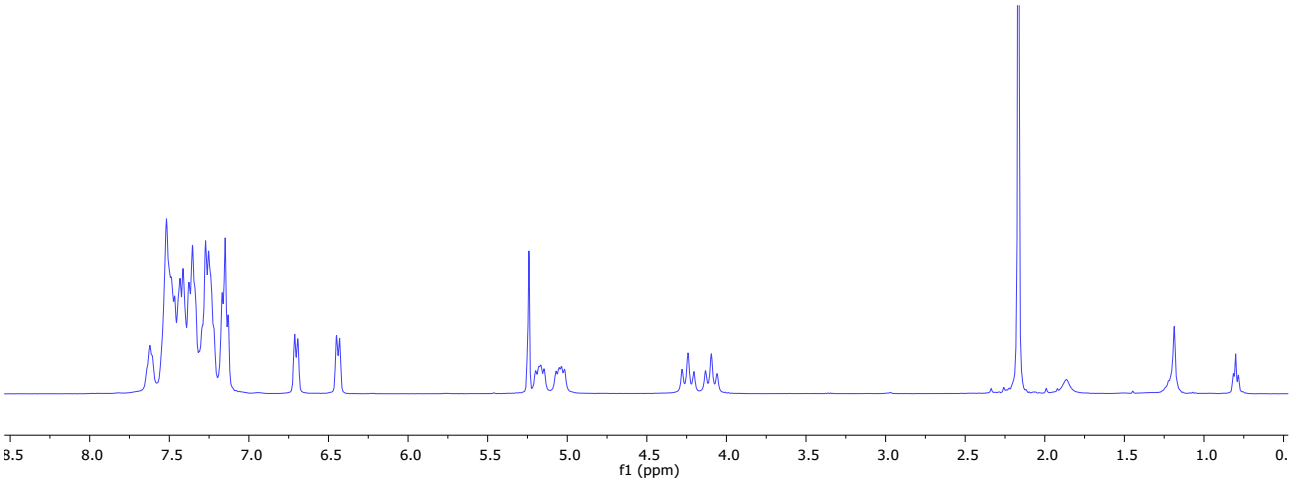
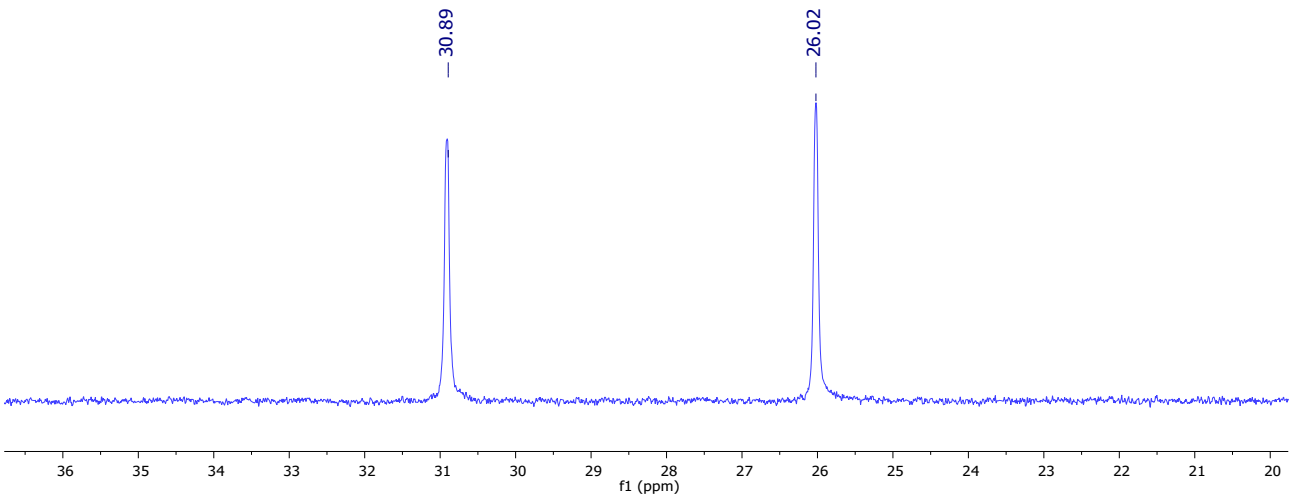


Figure S20. NMR spectra of $(DPPMPY_2Au_4Cl_2)(BF_4)_2$, **5**

^{1}H NMR



$^{31}P\{1H\}$ NMR



$^{13}C\{^{1}H\}$ NMR

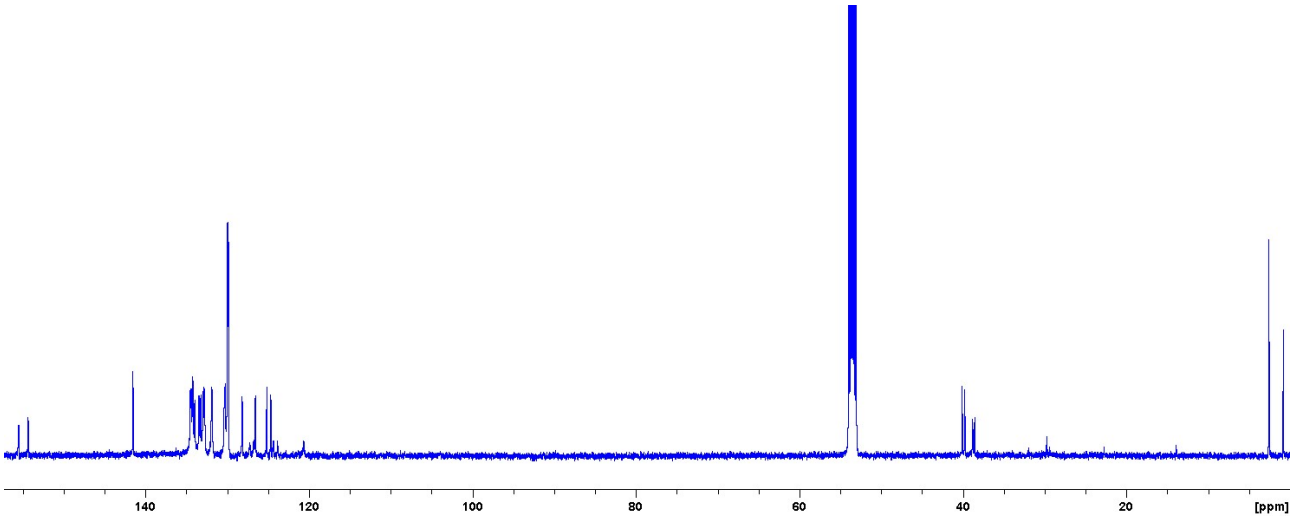
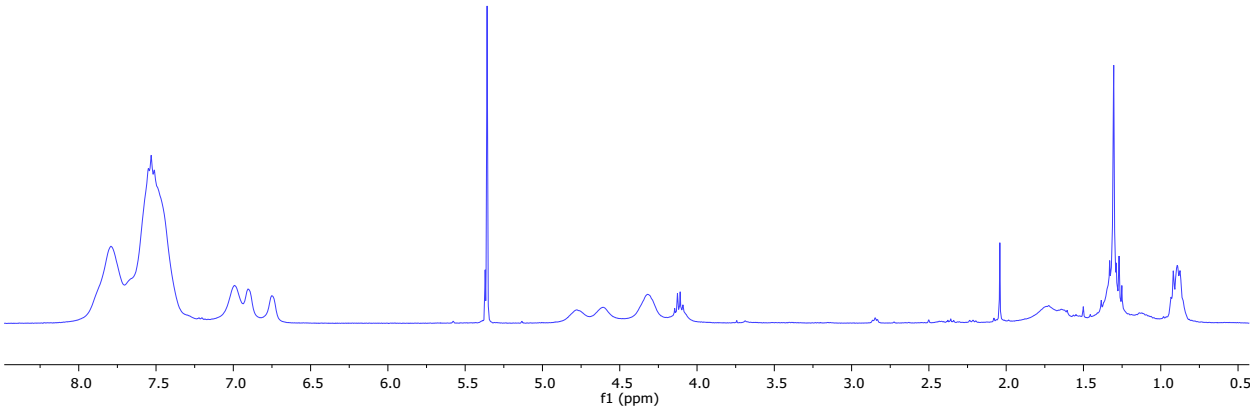
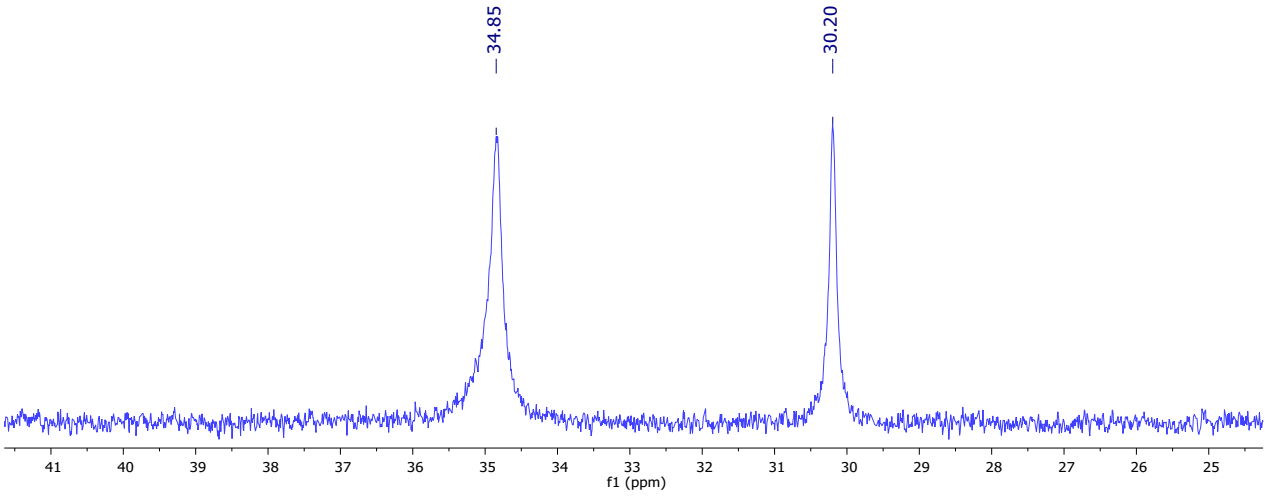


Figure S21. NMR spectra of $(DPPMPY_2Au4(MeCN)_2)(BF_4)_4$, **6**

^{1}H NMR



$^{31}P\{1H\}$ NMR



$^{13}C\{^{1}H\}$ NMR

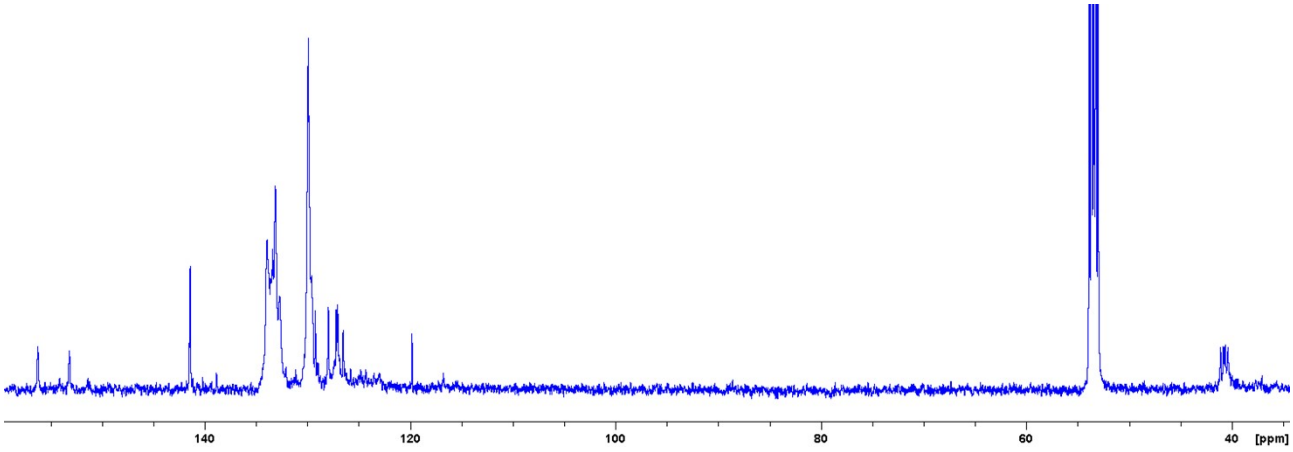


Figure S22. NMR spectra of $(DPPMPY_2Au_4Br_2)(BF_4)_2$, **7**

VIII. X-RAY data

Complex 1

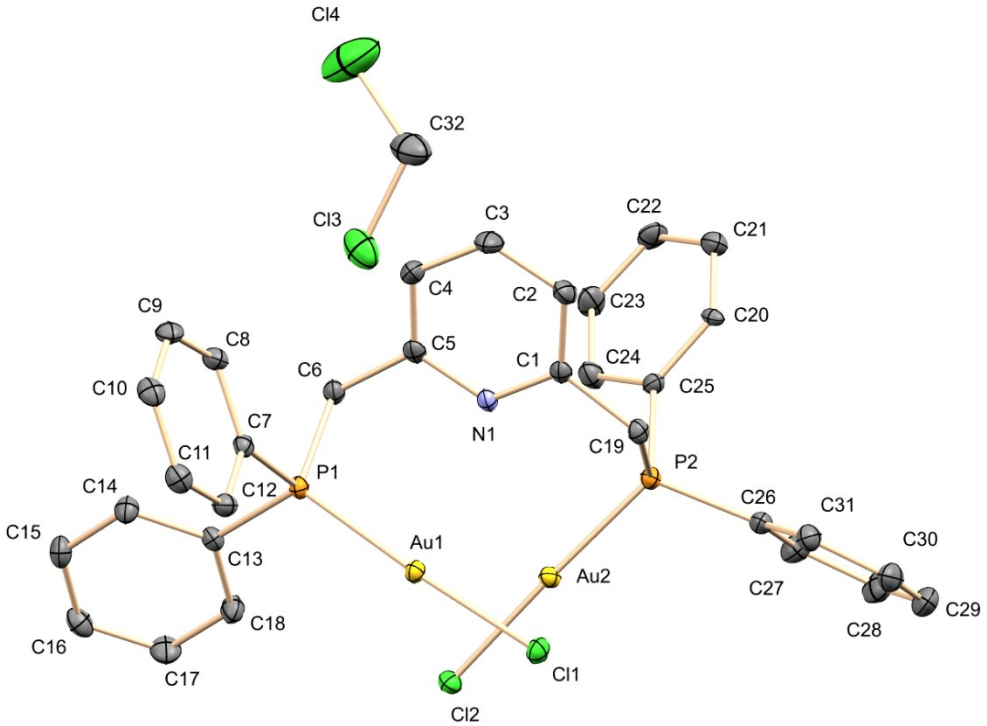


Table 1. Crystal data and structure refinement for **Complex 1**.

Identification code	**Complex 1**	
Empirical formula	C31.50 H28 Au2 Cl3 N P2	
Formula weight	982.77	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.9762(4) Å	α= 90.049(2)°.
	b = 12.4423(5) Å	β= 95.592(2)°.
	c = 14.4881(7) Å	γ = 107.456(2)°.
Volume	1535.46(12) $Å^3$	
Z	2	
Density (calculated)	2.126 Mg/m^3	
Absorption coefficient	9.932 mm^{-1}	
F(000)	926	
Crystal size	0.13 x 0.105 x 0.085 mm^3	
Theta range for data collection	2.258 to 30.034°.	
Index ranges	-12<=h<=12, -17<=k<=17, -20<=l<=20	
Reflections collected	148921	
Independent reflections	8988 [R(int) = 0.0721]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7465 and 0.5249	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8988 / 24 / 370	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.0177, wR2 = 0.0355	
R indices (all data)	R1 = 0.0239, wR2 = 0.0369	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.717 and -0.953 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Complex 1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	6395(1)	7911(1)	1696(1)	11(1)
Au(2)	7439(1)	5900(1)	2897(1)	11(1)
Cl(1)	7848(1)	7165(1)	794(1)	15(1)
Cl(2)	9245(1)	7474(1)	3621(1)	15(1)
P(1)	4831(1)	8582(1)	2488(1)	11(1)
P(2)	5765(1)	4326(1)	2226(1)	11(1)
N(1)	3789(2)	5906(2)	2132(1)	12(1)
C(1)	3281(3)	5056(2)	1497(2)	12(1)
C(2)	1731(3)	4691(2)	1097(2)	17(1)
C(3)	693(3)	5242(2)	1352(2)	22(1)
C(4)	1223(3)	6133(2)	1999(2)	18(1)
C(5)	2777(3)	6434(2)	2377(2)	13(1)
C(6)	3490(3)	7420(2)	3054(2)	14(1)
C(7)	3613(3)	9256(2)	1777(2)	12(1)
C(8)	2023(3)	9076(2)	1869(2)	15(1)
C(9)	1183(3)	9664(2)	1328(2)	17(1)
C(10)	1914(3)	10435(2)	701(2)	18(1)
C(11)	3505(3)	10622(2)	613(2)	17(1)
C(12)	4347(3)	10035(2)	1144(2)	15(1)
C(13)	5808(3)	9626(2)	3398(2)	12(1)
C(14)	5111(3)	10416(2)	3676(2)	16(1)
C(15)	5898(3)	11237(2)	4347(2)	18(1)
C(16)	7373(3)	11272(2)	4748(2)	18(1)
C(17)	8049(3)	10470(2)	4493(2)	21(1)
C(18)	7286(3)	9650(2)	3809(2)	18(1)
C(19)	4492(3)	4545(2)	1224(2)	12(1)
C(20)	3323(2)	2489(2)	2706(2)	10(1)
C(21)	2260(3)	1869(2)	3265(2)	18(1)
C(22)	2264(3)	2280(2)	4152(2)	21(1)
C(23)	3338(3)	3294(2)	4467(2)	22(1)
C(24)	4411(3)	3906(2)	3889(2)	18(1)
C(25)	4414(3)	3498(2)	2992(2)	12(1)
C(26)	6752(3)	3390(2)	1778(2)	14(1)
C(27)	7574(3)	2878(2)	2418(2)	22(1)

C(28)	8419(3)	2202(3)	2116(2)	28(1)
C(29)	8467(3)	2039(2)	1175(2)	27(1)
C(30)	7660(3)	2536(2)	534(2)	24(1)
C(31)	6799(3)	3205(2)	832(2)	17(1)
Cl(3)	1806(5)	5650(3)	4921(3)	33(1)
Cl(4)	-1435(5)	4578(4)	5266(4)	70(1)
C(32)	68(6)	4593(5)	4562(5)	36(1)

Table 3. Bond lengths [Å] and angles [°] for **Complex 1**.

Au(1)-Cl(1)	2.3078(6)
Au(1)-P(1)	2.2365(6)
Au(2)-Cl(2)	2.3078(6)
Au(2)-P(2)	2.2320(6)
P(1)-C(6)	1.833(2)
P(1)-C(7)	1.815(2)
P(1)-C(13)	1.811(2)
P(2)-C(19)	1.830(2)
P(2)-C(25)	1.810(2)
P(2)-C(26)	1.815(2)
N(1)-C(1)	1.341(3)
N(1)-C(5)	1.343(3)
C(1)-C(2)	1.393(3)
C(1)-C(19)	1.498(3)
C(2)-H(2)	0.9500
C(2)-C(3)	1.388(4)
C(3)-H(3)	0.9500
C(3)-C(4)	1.389(4)
C(4)-H(4)	0.9500
C(4)-C(5)	1.387(3)
C(5)-C(6)	1.511(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.397(3)
C(7)-C(12)	1.397(3)
C(8)-H(8)	0.9500
C(8)-C(9)	1.392(3)

C(9)-H(9)	0.9500
C(9)-C(10)	1.384(4)
C(10)-H(10)	0.9500
C(10)-C(11)	1.394(4)
C(11)-H(11)	0.9500
C(11)-C(12)	1.385(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.392(3)
C(13)-C(18)	1.392(3)
C(14)-H(14)	0.9500
C(14)-C(15)	1.385(3)
C(15)-H(15)	0.9500
C(15)-C(16)	1.381(4)
C(16)-H(16)	0.9500
C(16)-C(17)	1.381(4)
C(17)-H(17)	0.9500
C(17)-C(18)	1.392(4)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20)	0.9500
C(20)-C(21)	1.369(3)
C(20)-C(25)	1.375(3)
C(21)-H(21)	0.9500
C(21)-C(22)	1.382(4)
C(22)-H(22)	0.9500
C(22)-C(23)	1.383(4)
C(23)-H(23)	0.9500
C(23)-C(24)	1.389(3)
C(24)-H(24)	0.9500
C(24)-C(25)	1.395(3)
C(26)-C(27)	1.399(4)
C(26)-C(31)	1.396(3)
C(27)-H(27)	0.9500
C(27)-C(28)	1.386(4)
C(28)-H(28)	0.9500
C(28)-C(29)	1.386(4)
C(29)-H(29)	0.9500
C(29)-C(30)	1.381(4)

C(30)-H(30)	0.9500
C(30)-C(31)	1.389(4)
C(31)-H(31)	0.9500
Cl(3)-C(32)	1.745(6)
Cl(4)-C(32)	1.765(7)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900

P(1)-Au(1)-Cl(1)	175.59(2)
P(2)-Au(2)-Cl(2)	177.17(2)
C(6)-P(1)-Au(1)	109.46(8)
C(7)-P(1)-Au(1)	114.16(8)
C(7)-P(1)-C(6)	106.56(11)
C(13)-P(1)-Au(1)	115.94(8)
C(13)-P(1)-C(6)	106.05(11)
C(13)-P(1)-C(7)	103.95(11)
C(19)-P(2)-Au(2)	114.95(8)
C(25)-P(2)-Au(2)	113.83(8)
C(25)-P(2)-C(19)	104.12(11)
C(25)-P(2)-C(26)	106.21(11)
C(26)-P(2)-Au(2)	112.70(8)
C(26)-P(2)-C(19)	104.04(11)
C(1)-N(1)-C(5)	118.8(2)
N(1)-C(1)-C(2)	122.2(2)
N(1)-C(1)-C(19)	115.9(2)
C(2)-C(1)-C(19)	121.9(2)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-C(1)	118.6(2)
C(3)-C(2)-H(2)	120.7
C(2)-C(3)-H(3)	120.3
C(2)-C(3)-C(4)	119.3(2)
C(4)-C(3)-H(3)	120.3
C(3)-C(4)-H(4)	120.7
C(5)-C(4)-C(3)	118.6(2)
C(5)-C(4)-H(4)	120.7
N(1)-C(5)-C(4)	122.5(2)
N(1)-C(5)-C(6)	114.6(2)
C(4)-C(5)-C(6)	122.8(2)
P(1)-C(6)-H(6A)	109.6

P(1)-C(6)-H(6B)	109.6
C(5)-C(6)-P(1)	110.15(16)
C(5)-C(6)-H(6A)	109.6
C(5)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
C(8)-C(7)-P(1)	123.25(18)
C(12)-C(7)-P(1)	117.25(18)
C(12)-C(7)-C(8)	119.4(2)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-C(7)	119.9(2)
C(9)-C(8)-H(8)	120.0
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-C(8)	120.5(2)
C(10)-C(9)-H(9)	119.8
C(9)-C(10)-H(10)	120.2
C(9)-C(10)-C(11)	119.6(2)
C(11)-C(10)-H(10)	120.2
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-C(10)	120.3(2)
C(12)-C(11)-H(11)	119.9
C(7)-C(12)-H(12)	119.9
C(11)-C(12)-C(7)	120.2(2)
C(11)-C(12)-H(12)	119.9
C(14)-C(13)-P(1)	120.74(18)
C(18)-C(13)-P(1)	119.49(18)
C(18)-C(13)-C(14)	119.8(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-C(13)	120.1(2)
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-H(15)	119.9
C(16)-C(15)-C(14)	120.2(2)
C(16)-C(15)-H(15)	119.9
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-C(15)	119.8(2)
C(17)-C(16)-H(16)	120.1
C(16)-C(17)-H(17)	119.7
C(16)-C(17)-C(18)	120.7(2)
C(18)-C(17)-H(17)	119.7
C(13)-C(18)-C(17)	119.3(2)

C(13)-C(18)-H(18)	120.3
C(17)-C(18)-H(18)	120.3
P(2)-C(19)-H(19A)	109.1
P(2)-C(19)-H(19B)	109.1
C(1)-C(19)-P(2)	112.28(16)
C(1)-C(19)-H(19A)	109.1
C(1)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.9
C(21)-C(20)-H(20)	118.6
C(21)-C(20)-C(25)	122.9(2)
C(25)-C(20)-H(20)	118.6
C(20)-C(21)-H(21)	120.6
C(20)-C(21)-C(22)	118.7(2)
C(22)-C(21)-H(21)	120.6
C(21)-C(22)-H(22)	119.8
C(21)-C(22)-C(23)	120.3(2)
C(23)-C(22)-H(22)	119.8
C(22)-C(23)-H(23)	120.0
C(22)-C(23)-C(24)	119.9(2)
C(24)-C(23)-H(23)	120.0
C(23)-C(24)-H(24)	119.9
C(23)-C(24)-C(25)	120.1(2)
C(25)-C(24)-H(24)	119.9
C(20)-C(25)-P(2)	122.04(18)
C(20)-C(25)-C(24)	118.0(2)
C(24)-C(25)-P(2)	119.91(18)
C(27)-C(26)-P(2)	117.86(19)
C(31)-C(26)-P(2)	123.26(19)
C(31)-C(26)-C(27)	118.8(2)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-C(26)	120.5(3)
C(28)-C(27)-H(27)	119.7
C(27)-C(28)-H(28)	120.1
C(29)-C(28)-C(27)	119.9(3)
C(29)-C(28)-H(28)	120.1
C(28)-C(29)-H(29)	119.8
C(30)-C(29)-C(28)	120.3(3)
C(30)-C(29)-H(29)	119.8
C(29)-C(30)-H(30)	120.0

C(29)-C(30)-C(31)	120.0(3)
C(31)-C(30)-H(30)	120.0
C(26)-C(31)-H(31)	119.8
C(30)-C(31)-C(26)	120.4(2)
C(30)-C(31)-H(31)	119.8
Cl(3)-C(32)-Cl(4)	111.8(4)
Cl(3)-C(32)-H(32A)	109.3
Cl(3)-C(32)-H(32B)	109.3
Cl(4)-C(32)-H(32A)	109.3
Cl(4)-C(32)-H(32B)	109.3
H(32A)-C(32)-H(32B)	107.9

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Complex 1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	13(1)	11(1)	11(1)	-1(1)	2(1)	4(1)
Au(2)	11(1)	12(1)	10(1)	-1(1)	1(1)	2(1)
Cl(1)	18(1)	16(1)	13(1)	-1(1)	5(1)	6(1)
Cl(2)	12(1)	15(1)	17(1)	-4(1)	1(1)	2(1)
P(1)	12(1)	10(1)	10(1)	-1(1)	1(1)	4(1)
P(2)	12(1)	12(1)	9(1)	-1(1)	1(1)	3(1)
N(1)	14(1)	9(1)	11(1)	-1(1)	2(1)	3(1)
C(1)	14(1)	10(1)	11(1)	2(1)	4(1)	3(1)
C(2)	15(1)	16(1)	18(1)	-6(1)	2(1)	0(1)
C(3)	11(1)	24(1)	29(2)	-8(1)	1(1)	1(1)
C(4)	14(1)	16(1)	25(1)	-4(1)	6(1)	3(1)
C(5)	16(1)	10(1)	11(1)	2(1)	6(1)	2(1)
C(6)	16(1)	11(1)	14(1)	0(1)	3(1)	4(1)
C(7)	13(1)	12(1)	11(1)	-3(1)	-1(1)	3(1)
C(8)	13(1)	15(1)	16(1)	0(1)	2(1)	1(1)
C(9)	11(1)	18(1)	21(1)	-1(1)	-1(1)	2(1)
C(10)	19(1)	17(1)	16(1)	-1(1)	-5(1)	5(1)
C(11)	21(1)	16(1)	13(1)	1(1)	1(1)	4(1)
C(12)	13(1)	17(1)	14(1)	-2(1)	2(1)	2(1)
C(13)	14(1)	10(1)	11(1)	0(1)	1(1)	2(1)

C(14)	16(1)	17(1)	16(1)	-3(1)	-2(1)	8(1)
C(15)	24(1)	15(1)	17(1)	-3(1)	2(1)	9(1)
C(16)	22(1)	16(1)	14(1)	-2(1)	-2(1)	2(1)
C(17)	16(1)	24(1)	23(1)	-3(1)	-6(1)	6(1)
C(18)	17(1)	17(1)	22(1)	-4(1)	-2(1)	9(1)
C(19)	15(1)	13(1)	9(1)	-2(1)	1(1)	4(1)
C(20)	6(1)	9(1)	12(1)	3(1)	-1(1)	1(1)
C(21)	15(1)	15(1)	25(1)	1(1)	4(1)	2(1)
C(22)	21(1)	20(1)	24(1)	6(1)	13(1)	7(1)
C(23)	28(1)	22(1)	17(1)	-1(1)	11(1)	5(1)
C(24)	21(1)	15(1)	16(1)	-2(1)	4(1)	2(1)
C(25)	11(1)	12(1)	14(1)	1(1)	4(1)	4(1)
C(26)	13(1)	11(1)	17(1)	0(1)	4(1)	2(1)
C(27)	22(1)	29(1)	22(1)	5(1)	5(1)	13(1)
C(28)	25(1)	29(2)	36(2)	9(1)	6(1)	17(1)
C(29)	20(1)	21(1)	43(2)	-3(1)	9(1)	9(1)
C(30)	22(1)	23(1)	25(1)	-9(1)	8(1)	3(1)
C(31)	17(1)	17(1)	17(1)	-3(1)	1(1)	4(1)
Cl(3)	40(2)	22(1)	34(1)	5(1)	-4(1)	8(1)
Cl(4)	55(3)	78(3)	100(4)	54(2)	43(2)	43(2)
C(32)	24(3)	32(3)	46(4)	4(3)	-3(3)	4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **Complex 1**.

	x	y	z	U(eq)
H(2)	1392	4077	658	21
H(3)	-369	5012	1088	27
H(4)	535	6528	2179	22
H(6A)	4070	7183	3593	16
H(6B)	2646	7677	3284	16
H(8)	1515	8551	2301	18
H(9)	100	9536	1389	20
H(10)	1336	10834	332	21
H(11)	4012	11155	187	20
H(12)	5429	10163	1078	18
H(14)	4093	10392	3406	19
H(15)	5422	11778	4532	22
H(16)	7921	11846	5198	22
H(17)	9046	10478	4787	25
H(18)	7768	9112	3625	22
H(19A)	5144	5045	790	15
H(19B)	3960	3812	895	15
H(20)	3306	2210	2093	12
H(21)	1533	1168	3048	22
H(22)	1527	1865	4547	25
H(23)	3341	3572	5078	27
H(24)	5146	4605	4104	21
H(27)	7553	2995	3064	27
H(28)	8964	1850	2555	33
H(29)	9057	1583	969	32
H(30)	7695	2420	-111	29
H(31)	6237	3540	389	21
H(32A)	267	3852	4584	43
H(32B)	-280	4713	3911	43

Table 6. Torsion angles [°] for **Complex 1**.

Au(1)-P(1)-C(6)-C(5)	-46.53(18)
Au(1)-P(1)-C(7)-C(8)	135.85(18)
Au(1)-P(1)-C(7)-C(12)	-47.6(2)
Au(1)-P(1)-C(13)-C(14)	153.89(17)
Au(1)-P(1)-C(13)-C(18)	-24.9(2)
Au(2)-P(2)-C(19)-C(1)	-70.69(17)
Au(2)-P(2)-C(25)-C(20)	-178.45(17)
Au(2)-P(2)-C(25)-C(24)	4.6(2)
Au(2)-P(2)-C(26)-C(27)	67.5(2)
Au(2)-P(2)-C(26)-C(31)	-109.0(2)
P(1)-C(7)-C(8)-C(9)	176.99(19)
P(1)-C(7)-C(12)-C(11)	-176.78(19)
P(1)-C(13)-C(14)-C(15)	-177.45(19)
P(1)-C(13)-C(18)-C(17)	178.5(2)
P(2)-C(26)-C(27)-C(28)	-176.6(2)
P(2)-C(26)-C(31)-C(30)	175.8(2)
N(1)-C(1)-C(2)-C(3)	1.3(4)
N(1)-C(1)-C(19)-P(2)	43.5(3)
N(1)-C(5)-C(6)-P(1)	69.2(2)
C(1)-N(1)-C(5)-C(4)	0.2(3)
C(1)-N(1)-C(5)-C(6)	-176.6(2)
C(1)-C(2)-C(3)-C(4)	-0.3(4)
C(2)-C(1)-C(19)-P(2)	-138.2(2)
C(2)-C(3)-C(4)-C(5)	-0.7(4)
C(3)-C(4)-C(5)-N(1)	0.8(4)
C(3)-C(4)-C(5)-C(6)	177.3(2)
C(4)-C(5)-C(6)-P(1)	-107.5(2)
C(5)-N(1)-C(1)-C(2)	-1.3(3)
C(5)-N(1)-C(1)-C(19)	177.1(2)
C(6)-P(1)-C(7)-C(8)	14.9(2)
C(6)-P(1)-C(7)-C(12)	-168.51(18)
C(6)-P(1)-C(13)-C(14)	-84.4(2)
C(6)-P(1)-C(13)-C(18)	96.8(2)
C(7)-P(1)-C(6)-C(5)	77.38(18)
C(7)-P(1)-C(13)-C(14)	27.7(2)
C(7)-P(1)-C(13)-C(18)	-151.0(2)
C(7)-C(8)-C(9)-C(10)	-0.4(4)

C(8)-C(7)-C(12)-C(11)	0.0(4)
C(8)-C(9)-C(10)-C(11)	-0.1(4)
C(9)-C(10)-C(11)-C(12)	0.5(4)
C(10)-C(11)-C(12)-C(7)	-0.4(4)
C(12)-C(7)-C(8)-C(9)	0.5(4)
C(13)-P(1)-C(6)-C(5)	-172.30(16)
C(13)-P(1)-C(7)-C(8)	-96.9(2)
C(13)-P(1)-C(7)-C(12)	79.7(2)
C(13)-C(14)-C(15)-C(16)	-0.5(4)
C(14)-C(13)-C(18)-C(17)	-0.3(4)
C(14)-C(15)-C(16)-C(17)	-1.4(4)
C(15)-C(16)-C(17)-C(18)	2.5(4)
C(16)-C(17)-C(18)-C(13)	-1.6(4)
C(18)-C(13)-C(14)-C(15)	1.3(4)
C(19)-P(2)-C(25)-C(20)	55.6(2)
C(19)-P(2)-C(25)-C(24)	-121.3(2)
C(19)-P(2)-C(26)-C(27)	-167.3(2)
C(19)-P(2)-C(26)-C(31)	16.2(2)
C(19)-C(1)-C(2)-C(3)	-176.9(2)
C(20)-C(21)-C(22)-C(23)	-0.7(4)
C(21)-C(20)-C(25)-P(2)	-177.92(19)
C(21)-C(20)-C(25)-C(24)	-0.9(4)
C(21)-C(22)-C(23)-C(24)	0.4(4)
C(22)-C(23)-C(24)-C(25)	-0.3(4)
C(23)-C(24)-C(25)-P(2)	177.6(2)
C(23)-C(24)-C(25)-C(20)	0.5(4)
C(25)-P(2)-C(19)-C(1)	54.52(19)
C(25)-P(2)-C(26)-C(27)	-57.7(2)
C(25)-P(2)-C(26)-C(31)	125.7(2)
C(25)-C(20)-C(21)-C(22)	1.0(4)
C(26)-P(2)-C(19)-C(1)	165.60(16)
C(26)-P(2)-C(25)-C(20)	-53.9(2)
C(26)-P(2)-C(25)-C(24)	129.2(2)
C(26)-C(27)-C(28)-C(29)	0.7(4)
C(27)-C(26)-C(31)-C(30)	-0.7(4)
C(27)-C(28)-C(29)-C(30)	-0.8(4)
C(28)-C(29)-C(30)-C(31)	0.1(4)
C(29)-C(30)-C(31)-C(26)	0.6(4)
C(31)-C(26)-C(27)-C(28)	0.1(4)

Symmetry transformations used to generate equivalent atoms:

Complex 2

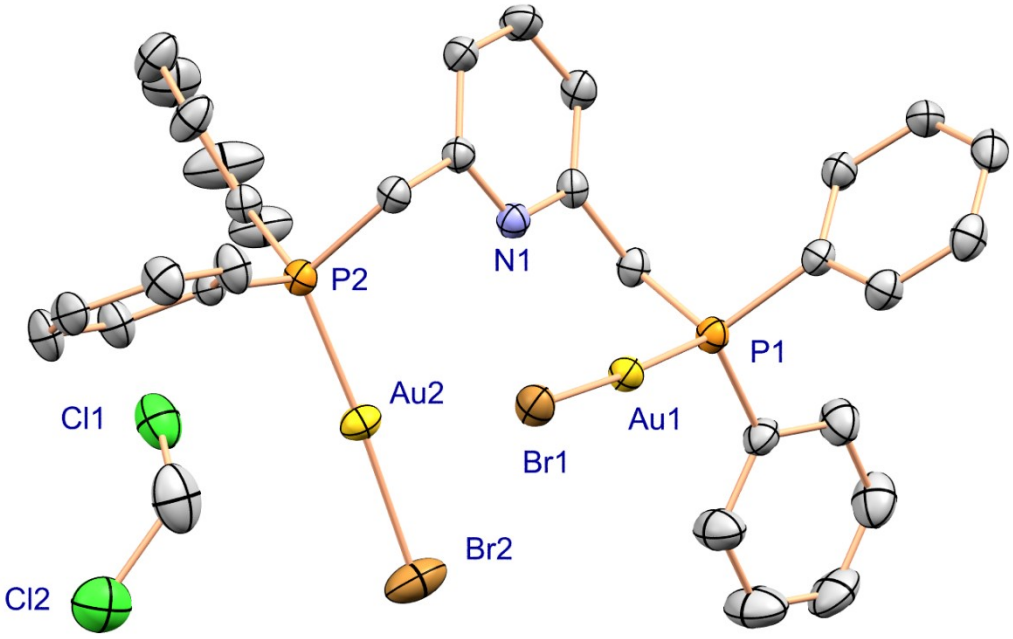


Table 1. Crystal data and structure refinement for **Complex 2**

Identification code	**Complex 2**	
Empirical formula	C32 H29 Au2 Br2 Cl2 N P2	
Formula weight	1114.15	
Temperature	150.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.7361(4) Å	α= 90°.
	b = 12.8876(3) Å	β= 90.4110(10)°.
	c = 16.5348(4) Å	γ = 90°.
Volume	3353.18(14) $Å^3$	
Z	4	
Density (calculated)	2.207 Mg/m^3	
Absorption coefficient	11.402 mm^{-1}	
F(000)	2080	
Crystal size	0.45 x 0.09 x 0.035 mm^3	
Theta range for data collection	2.381 to 30.080°.	
Index ranges	-22<=h<=22, -18<=k<=18, -23<=l<=23	
Reflections collected	91509	
Independent reflections	9836 [R(int) = 0.0579]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0990 and 0.0403	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9836 / 0 / 370	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0289, wR2 = 0.0691	
R indices (all data)	R1 = 0.0382, wR2 = 0.0732	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.755 and -1.748 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Complex 2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	1562(1)	7697(1)	5555(1)	24(1)
Au(2)	2781(1)	5219(1)	5951(1)	28(1)
Br(1)	713(1)	6614(1)	6423(1)	32(1)
Br(2)	3674(1)	6232(1)	6835(1)	50(1)
P(1)	2285(1)	8689(1)	4688(1)	23(1)
P(2)	2004(1)	4196(1)	5145(1)	22(1)
N(1)	1991(2)	6349(3)	4208(2)	23(1)
C(1)	1488(3)	5564(3)	3968(2)	23(1)
C(2)	1295(3)	5390(4)	3155(3)	30(1)
C(3)	1639(3)	6043(4)	2587(3)	34(1)
C(4)	2151(3)	6863(4)	2829(3)	28(1)
C(5)	2311(3)	6987(3)	3647(3)	23(1)
C(6)	2851(3)	7864(3)	3974(3)	24(1)
C(7)	3098(3)	9532(4)	5115(3)	28(1)
C(8)	3386(3)	10391(4)	4687(4)	39(1)
C(9)	4024(4)	11012(5)	5013(4)	48(1)
C(10)	4370(4)	10804(5)	5759(4)	52(2)
C(11)	4081(5)	9949(6)	6184(4)	59(2)
C(12)	3449(4)	9312(5)	5864(3)	46(1)
C(13)	1610(3)	9547(3)	4096(3)	24(1)
C(14)	1655(3)	9641(4)	3261(3)	29(1)
C(15)	1143(3)	10357(4)	2857(3)	32(1)
C(16)	585(3)	10976(4)	3278(3)	34(1)
C(17)	532(3)	10878(4)	4122(3)	33(1)
C(18)	1036(3)	10174(4)	4524(3)	29(1)
C(19)	1141(3)	4876(3)	4621(3)	24(1)
C(20)	2588(3)	3602(3)	4322(3)	26(1)
C(21)	2204(4)	2836(4)	3848(3)	36(1)
C(22)	2615(4)	2454(4)	3177(3)	42(1)
C(23)	3415(4)	2811(5)	2987(4)	51(2)
C(24)	3791(4)	3569(7)	3449(4)	64(2)
C(25)	3382(3)	3975(5)	4120(3)	46(1)
C(26)	1481(3)	3148(3)	5679(2)	24(1)
C(27)	623(3)	3189(4)	5858(3)	35(1)

C(28)	238(3)	2397(4)	6290(3)	37(1)
C(29)	710(4)	1567(4)	6550(3)	36(1)
C(30)	1573(4)	1518(4)	6384(3)	41(1)
C(31)	1960(3)	2318(4)	5957(3)	36(1)
Cl(1)	5346(1)	3605(1)	5143(1)	51(1)
Cl(2)	5342(1)	3295(2)	6900(1)	59(1)
C(32)	4806(4)	3809(6)	6051(5)	60(2)

Table 3. Bond lengths [Å] and angles [°] for **Complex 2**

Au(1)-Br(1)	2.4127(5)
Au(1)-P(1)	2.2387(11)
Au(2)-Br(2)	2.4058(6)
Au(2)-P(2)	2.2323(11)
P(1)-C(6)	1.824(4)
P(1)-C(7)	1.818(5)
P(1)-C(13)	1.815(4)
P(2)-C(19)	1.828(4)
P(2)-C(20)	1.817(4)
P(2)-C(26)	1.814(4)
N(1)-C(1)	1.342(6)
N(1)-C(5)	1.340(5)
C(1)-C(2)	1.395(6)
C(1)-C(19)	1.503(6)
C(2)-H(2)	0.9500
C(2)-C(3)	1.375(7)
C(3)-H(3)	0.9500
C(3)-C(4)	1.386(7)
C(4)-H(4)	0.9500
C(4)-C(5)	1.383(6)
C(5)-C(6)	1.513(6)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.391(7)
C(7)-C(12)	1.382(7)
C(8)-H(8)	0.9500
C(8)-C(9)	1.389(8)
C(9)-H(9)	0.9500
C(9)-C(10)	1.372(9)
C(10)-H(10)	0.9500
C(10)-C(11)	1.384(10)
C(11)-H(11)	0.9500
C(11)-C(12)	1.391(8)
C(12)-H(12)	0.9500
C(13)-C(14)	1.388(6)
C(13)-C(18)	1.407(6)
C(14)-H(14)	0.9500

C(14)-C(15)	1.393(7)
C(15)-H(15)	0.9500
C(15)-C(16)	1.378(7)
C(16)-H(16)	0.9500
C(16)-C(17)	1.404(7)
C(17)-H(17)	0.9500
C(17)-C(18)	1.373(7)
C(18)-H(18)	0.9500
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.395(7)
C(20)-C(25)	1.383(7)
C(21)-H(21)	0.9500
C(21)-C(22)	1.380(7)
C(22)-H(22)	0.9500
C(22)-C(23)	1.379(8)
C(23)-H(23)	0.9500
C(23)-C(24)	1.372(9)
C(24)-H(24)	0.9500
C(24)-C(25)	1.389(8)
C(25)-H(25)	0.9500
C(26)-C(27)	1.385(6)
C(26)-C(31)	1.385(7)
C(27)-H(27)	0.9500
C(27)-C(28)	1.388(7)
C(28)-H(28)	0.9500
C(28)-C(29)	1.370(7)
C(29)-H(29)	0.9500
C(29)-C(30)	1.389(8)
C(30)-H(30)	0.9500
C(30)-C(31)	1.392(7)
C(31)-H(31)	0.9500
Cl(1)-C(32)	1.749(7)
Cl(2)-C(32)	1.763(7)
C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900

P(1)-Au(1)-Br(1)	176.30(3)
P(2)-Au(2)-Br(2)	176.50(3)

C(6)-P(1)-Au(1)	109.49(14)
C(7)-P(1)-Au(1)	116.87(16)
C(7)-P(1)-C(6)	104.8(2)
C(13)-P(1)-Au(1)	113.26(15)
C(13)-P(1)-C(6)	107.0(2)
C(13)-P(1)-C(7)	104.7(2)
C(19)-P(2)-Au(2)	113.69(15)
C(20)-P(2)-Au(2)	114.72(15)
C(20)-P(2)-C(19)	103.0(2)
C(26)-P(2)-Au(2)	113.39(14)
C(26)-P(2)-C(19)	104.4(2)
C(26)-P(2)-C(20)	106.5(2)
C(5)-N(1)-C(1)	118.8(4)
N(1)-C(1)-C(2)	122.0(4)
N(1)-C(1)-C(19)	116.7(4)
C(2)-C(1)-C(19)	121.3(4)
C(1)-C(2)-H(2)	120.8
C(3)-C(2)-C(1)	118.4(4)
C(3)-C(2)-H(2)	120.8
C(2)-C(3)-H(3)	120.0
C(2)-C(3)-C(4)	120.1(4)
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-H(4)	120.9
C(5)-C(4)-C(3)	118.1(4)
C(5)-C(4)-H(4)	120.9
N(1)-C(5)-C(4)	122.7(4)
N(1)-C(5)-C(6)	115.1(4)
C(4)-C(5)-C(6)	122.3(4)
P(1)-C(6)-H(6A)	109.0
P(1)-C(6)-H(6B)	109.0
C(5)-C(6)-P(1)	113.1(3)
C(5)-C(6)-H(6A)	109.0
C(5)-C(6)-H(6B)	109.0
H(6A)-C(6)-H(6B)	107.8
C(8)-C(7)-P(1)	120.6(4)
C(12)-C(7)-P(1)	120.1(4)
C(12)-C(7)-C(8)	119.3(5)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-C(7)	119.9(5)

C(9)-C(8)-H(8)	120.1
C(8)-C(9)-H(9)	119.4
C(10)-C(9)-C(8)	121.1(6)
C(10)-C(9)-H(9)	119.4
C(9)-C(10)-H(10)	120.6
C(9)-C(10)-C(11)	118.8(5)
C(11)-C(10)-H(10)	120.6
C(10)-C(11)-H(11)	119.5
C(10)-C(11)-C(12)	120.9(6)
C(12)-C(11)-H(11)	119.5
C(7)-C(12)-C(11)	119.9(6)
C(7)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-P(1)	123.7(3)
C(14)-C(13)-C(18)	119.2(4)
C(18)-C(13)-P(1)	117.0(3)
C(13)-C(14)-H(14)	120.0
C(13)-C(14)-C(15)	120.1(4)
C(15)-C(14)-H(14)	120.0
C(14)-C(15)-H(15)	119.7
C(16)-C(15)-C(14)	120.6(4)
C(16)-C(15)-H(15)	119.7
C(15)-C(16)-H(16)	120.2
C(15)-C(16)-C(17)	119.5(4)
C(17)-C(16)-H(16)	120.2
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-C(16)	120.1(4)
C(18)-C(17)-H(17)	119.9
C(13)-C(18)-H(18)	119.8
C(17)-C(18)-C(13)	120.4(4)
C(17)-C(18)-H(18)	119.8
P(2)-C(19)-H(19A)	109.5
P(2)-C(19)-H(19B)	109.5
C(1)-C(19)-P(2)	110.6(3)
C(1)-C(19)-H(19A)	109.5
C(1)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	108.1
C(21)-C(20)-P(2)	120.0(3)
C(25)-C(20)-P(2)	119.8(4)

C(25)-C(20)-C(21)	119.9(4)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-C(20)	120.1(5)
C(22)-C(21)-H(21)	119.9
C(21)-C(22)-H(22)	120.1
C(23)-C(22)-C(21)	119.8(5)
C(23)-C(22)-H(22)	120.1
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-C(22)	120.2(5)
C(24)-C(23)-H(23)	119.9
C(23)-C(24)-H(24)	119.6
C(23)-C(24)-C(25)	120.8(6)
C(25)-C(24)-H(24)	119.6
C(20)-C(25)-C(24)	119.1(5)
C(20)-C(25)-H(25)	120.4
C(24)-C(25)-H(25)	120.4
C(27)-C(26)-P(2)	121.5(3)
C(31)-C(26)-P(2)	119.3(4)
C(31)-C(26)-C(27)	119.1(4)
C(26)-C(27)-H(27)	119.6
C(26)-C(27)-C(28)	120.8(5)
C(28)-C(27)-H(27)	119.6
C(27)-C(28)-H(28)	120.1
C(29)-C(28)-C(27)	119.9(5)
C(29)-C(28)-H(28)	120.1
C(28)-C(29)-H(29)	119.9
C(28)-C(29)-C(30)	120.2(5)
C(30)-C(29)-H(29)	119.9
C(29)-C(30)-H(30)	120.1
C(29)-C(30)-C(31)	119.9(5)
C(31)-C(30)-H(30)	120.1
C(26)-C(31)-C(30)	120.1(5)
C(26)-C(31)-H(31)	119.9
C(30)-C(31)-H(31)	119.9
Cl(1)-C(32)-Cl(2)	113.2(3)
Cl(1)-C(32)-H(32A)	108.9
Cl(1)-C(32)-H(32B)	108.9
Cl(2)-C(32)-H(32A)	108.9
Cl(2)-C(32)-H(32B)	108.9

H(32A)-C(32)-H(32B) 107.7

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Complex 2** The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	28(1)	24(1)	21(1)	1(1)	3(1)	-2(1)
Au(2)	25(1)	31(1)	29(1)	-6(1)	1(1)	-3(1)
Br(1)	39(1)	30(1)	28(1)	2(1)	6(1)	-3(1)
Br(2)	33(1)	65(1)	53(1)	-31(1)	3(1)	-5(1)
P(1)	25(1)	21(1)	23(1)	1(1)	2(1)	-1(1)
P(2)	22(1)	22(1)	23(1)	1(1)	2(1)	-1(1)
N(1)	26(2)	21(2)	22(2)	0(1)	2(1)	2(1)
C(1)	25(2)	21(2)	24(2)	0(2)	1(2)	2(2)
C(2)	41(3)	23(2)	25(2)	-1(2)	-2(2)	-2(2)
C(3)	46(3)	32(2)	22(2)	0(2)	1(2)	-5(2)
C(4)	32(2)	25(2)	26(2)	1(2)	7(2)	-1(2)
C(5)	24(2)	19(2)	26(2)	2(2)	4(2)	2(2)
C(6)	24(2)	22(2)	27(2)	0(2)	4(2)	0(2)
C(7)	28(2)	23(2)	34(2)	-4(2)	-3(2)	-4(2)
C(8)	38(3)	31(3)	48(3)	6(2)	-5(2)	-6(2)
C(9)	35(3)	36(3)	72(4)	3(3)	-3(3)	-7(2)
C(10)	45(3)	43(3)	68(4)	-19(3)	-8(3)	-12(3)
C(11)	57(4)	72(5)	48(3)	-3(3)	-16(3)	-22(3)
C(12)	51(3)	49(3)	39(3)	3(2)	-9(2)	-14(3)
C(13)	25(2)	21(2)	26(2)	-2(2)	0(2)	-2(2)
C(14)	34(2)	24(2)	28(2)	-2(2)	1(2)	4(2)
C(15)	43(3)	27(2)	26(2)	-1(2)	-4(2)	1(2)
C(16)	31(2)	26(2)	46(3)	1(2)	-8(2)	0(2)
C(17)	27(2)	28(2)	43(3)	-4(2)	6(2)	2(2)
C(18)	28(2)	29(2)	30(2)	-2(2)	5(2)	1(2)
C(19)	24(2)	23(2)	24(2)	0(2)	2(2)	-1(2)
C(20)	25(2)	25(2)	26(2)	2(2)	3(2)	1(2)
C(21)	44(3)	28(2)	38(3)	-6(2)	13(2)	-10(2)
C(22)	52(3)	33(3)	41(3)	-9(2)	12(2)	-4(2)

C(23)	45(3)	66(4)	42(3)	-14(3)	14(2)	8(3)
C(24)	34(3)	113(6)	46(3)	-29(4)	13(3)	-17(3)
C(25)	30(3)	71(4)	37(3)	-16(3)	5(2)	-10(3)
C(26)	31(2)	21(2)	20(2)	2(2)	-1(2)	-6(2)
C(27)	33(2)	32(3)	41(3)	11(2)	6(2)	1(2)
C(28)	34(3)	37(3)	41(3)	10(2)	4(2)	-8(2)
C(29)	50(3)	27(2)	30(2)	10(2)	1(2)	-10(2)
C(30)	49(3)	31(3)	43(3)	16(2)	1(2)	4(2)
C(31)	38(3)	32(2)	37(2)	10(2)	3(2)	3(2)
Cl(1)	43(1)	49(1)	60(1)	11(1)	-3(1)	7(1)
Cl(2)	49(1)	73(1)	55(1)	-6(1)	9(1)	7(1)
C(32)	41(3)	59(4)	81(5)	11(4)	16(3)	19(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **Complex 2**

	x	y	z	U(eq)
H(2)	936	4832	2997	36
H(3)	1526	5933	2029	40
H(4)	2386	7326	2444	33
H(6A)	3049	8295	3517	29
H(6B)	3358	7569	4247	29
H(8)	3148	10552	4173	47
H(9)	4224	11591	4714	57
H(10)	4800	11238	5981	62
H(11)	4318	9796	6700	71
H(12)	3259	8726	6161	55
H(14)	2037	9217	2965	34
H(15)	1178	10419	2286	39
H(16)	239	11464	3000	41
H(17)	148	11301	4416	39
H(18)	996	10110	5095	35
H(19A)	746	4363	4380	29
H(19B)	820	5300	5014	29
H(21)	1659	2578	3987	44
H(22)	2347	1946	2846	50
H(23)	3707	2532	2536	61
H(24)	4339	3820	3309	77
H(25)	3645	4503	4436	55
H(27)	294	3766	5682	42
H(28)	-352	2430	6406	45
H(29)	446	1024	6844	43
H(30)	1899	940	6563	49
H(31)	2553	2294	5855	43
H(32A)	4236	3487	6010	73
H(32B)	4725	4564	6130	73

Table 6. Torsion angles [°] for **Complex 2**

Au(1)-P(1)-C(6)-C(5)	44.8(3)
Au(1)-P(1)-C(7)-C(8)	-159.5(4)
Au(1)-P(1)-C(7)-C(12)	21.9(5)
Au(1)-P(1)-C(13)-C(14)	-130.6(4)
Au(1)-P(1)-C(13)-C(18)	51.9(4)
Au(2)-P(2)-C(19)-C(1)	72.3(3)
Au(2)-P(2)-C(20)-C(21)	171.0(4)
Au(2)-P(2)-C(20)-C(25)	-15.0(5)
Au(2)-P(2)-C(26)-C(27)	102.8(4)
Au(2)-P(2)-C(26)-C(31)	-73.3(4)
P(1)-C(7)-C(8)-C(9)	-178.3(4)
P(1)-C(7)-C(12)-C(11)	178.9(5)
P(1)-C(13)-C(14)-C(15)	-176.8(4)
P(1)-C(13)-C(18)-C(17)	176.9(4)
P(2)-C(20)-C(21)-C(22)	173.9(4)
P(2)-C(20)-C(25)-C(24)	-174.8(5)
P(2)-C(26)-C(27)-C(28)	-177.8(4)
P(2)-C(26)-C(31)-C(30)	178.5(4)
N(1)-C(1)-C(2)-C(3)	0.3(7)
N(1)-C(1)-C(19)-P(2)	-63.6(4)
N(1)-C(5)-C(6)-P(1)	-57.9(5)
C(1)-N(1)-C(5)-C(4)	-0.8(6)
C(1)-N(1)-C(5)-C(6)	178.4(4)
C(1)-C(2)-C(3)-C(4)	-1.1(8)
C(2)-C(1)-C(19)-P(2)	116.1(4)
C(2)-C(3)-C(4)-C(5)	0.9(7)
C(3)-C(4)-C(5)-N(1)	0.0(7)
C(3)-C(4)-C(5)-C(6)	-179.1(4)
C(4)-C(5)-C(6)-P(1)	121.3(4)
C(5)-N(1)-C(1)-C(2)	0.7(6)
C(5)-N(1)-C(1)-C(19)	-179.6(4)
C(6)-P(1)-C(7)-C(8)	79.1(5)
C(6)-P(1)-C(7)-C(12)	-99.5(5)
C(6)-P(1)-C(13)-C(14)	-9.9(4)
C(6)-P(1)-C(13)-C(18)	172.7(3)
C(7)-P(1)-C(6)-C(5)	170.9(3)
C(7)-P(1)-C(13)-C(14)	101.0(4)

C(7)-P(1)-C(13)-C(18)	-76.5(4)
C(7)-C(8)-C(9)-C(10)	-0.9(9)
C(8)-C(7)-C(12)-C(11)	0.3(9)
C(8)-C(9)-C(10)-C(11)	0.9(10)
C(9)-C(10)-C(11)-C(12)	-0.2(11)
C(10)-C(11)-C(12)-C(7)	-0.4(11)
C(12)-C(7)-C(8)-C(9)	0.3(8)
C(13)-P(1)-C(6)-C(5)	-78.4(3)
C(13)-P(1)-C(7)-C(8)	-33.4(5)
C(13)-P(1)-C(7)-C(12)	148.0(4)
C(13)-C(14)-C(15)-C(16)	-0.2(7)
C(14)-C(13)-C(18)-C(17)	-0.7(7)
C(14)-C(15)-C(16)-C(17)	-0.3(7)
C(15)-C(16)-C(17)-C(18)	0.2(7)
C(16)-C(17)-C(18)-C(13)	0.2(7)
C(18)-C(13)-C(14)-C(15)	0.7(7)
C(19)-P(2)-C(20)-C(21)	-65.0(4)
C(19)-P(2)-C(20)-C(25)	109.1(5)
C(19)-P(2)-C(26)-C(27)	-21.5(4)
C(19)-P(2)-C(26)-C(31)	162.4(4)
C(19)-C(1)-C(2)-C(3)	-179.4(4)
C(20)-P(2)-C(19)-C(1)	-52.4(3)
C(20)-P(2)-C(26)-C(27)	-130.1(4)
C(20)-P(2)-C(26)-C(31)	53.8(4)
C(20)-C(21)-C(22)-C(23)	1.6(9)
C(21)-C(20)-C(25)-C(24)	-0.8(9)
C(21)-C(22)-C(23)-C(24)	-2.1(10)
C(22)-C(23)-C(24)-C(25)	1.1(12)
C(23)-C(24)-C(25)-C(20)	0.3(11)
C(25)-C(20)-C(21)-C(22)	-0.2(8)
C(26)-P(2)-C(19)-C(1)	-163.6(3)
C(26)-P(2)-C(20)-C(21)	44.6(4)
C(26)-P(2)-C(20)-C(25)	-141.3(4)
C(26)-C(27)-C(28)-C(29)	0.5(8)
C(27)-C(26)-C(31)-C(30)	2.3(8)
C(27)-C(28)-C(29)-C(30)	0.2(8)
C(28)-C(29)-C(30)-C(31)	0.3(8)
C(29)-C(30)-C(31)-C(26)	-1.6(8)
C(31)-C(26)-C(27)-C(28)	-1.7(8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **Complex 2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Complex 3

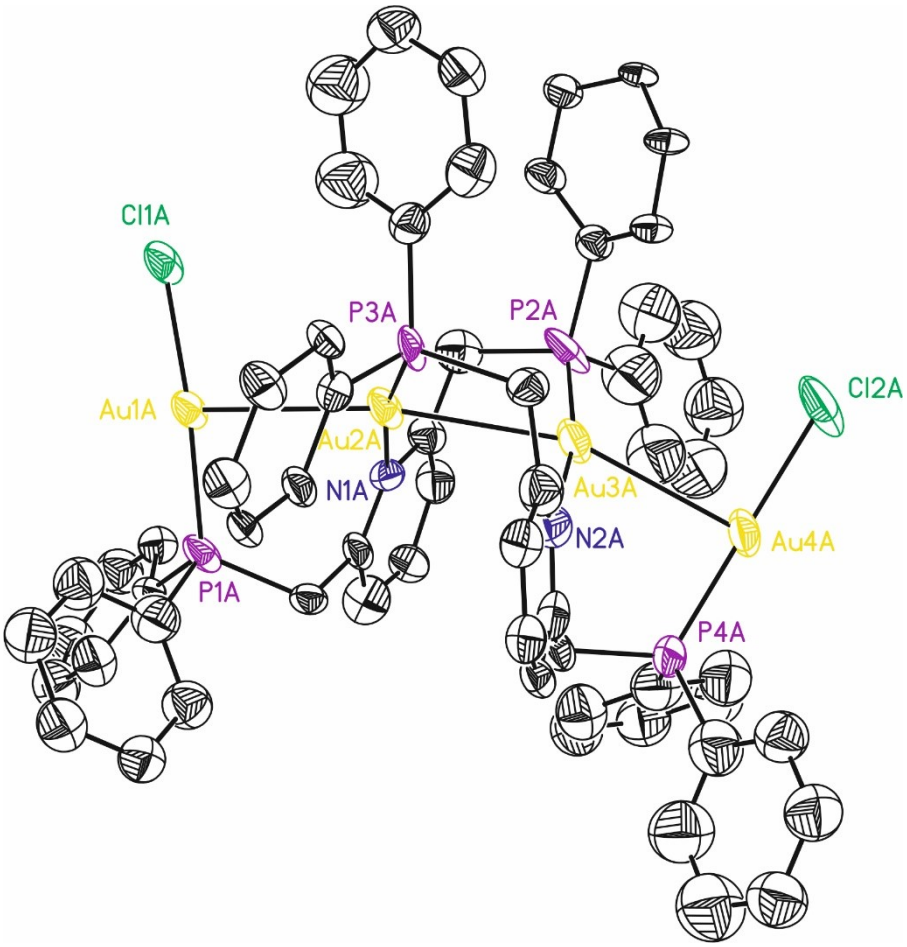


Table 1. Crystal data and structure refinement for **Complex 3**.

Identification code	**Complex 3**	
Empirical formula	C62 H54 Au4 Cl2 F12 N2 P4 Sb2	
Formula weight	2281.21	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 24.072(5)Å	α= 90°.
	b = 31.964(6)Å	β = 97.06(3)°.
	c = 20.304(4)Å	γ = 90°.
Volume	15504(5) $Å^3$	
Z	8	
Density (calculated)	1.955 Mg/m^3	
Absorption coefficient	8.444 mm^{-1}	
F(000)	8480	
Crystal size	0.100 x 0.050 x 0.005 mm^3	
Theta range for data collection	1.195 to 24.713°.	
Index ranges	-27<=h<=28,-37<=k<=37,-23<=l<=23	
Reflections collected	238149	
Independent reflections	26029[R(int) = 0.2414]	
Completeness to theta =24.713°	98.4%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.74 and 0.43	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26029/ 2558/ 1675	
Goodness-of-fit on F^2	1.588	
Final R indices [I>2sigma(I)]	R1 = 0.1273, wR2 = 0.3091	
R indices (all data)	R1 = 0.1927, wR2 = 0.3367	
Largest diff. peak and hole	5.675 and -3.959 $e.Å^{-3}$	

Table 2. Bond lengths [Å] and angles [°] for **Complex 3**.

Bond lengths----

Au1A P1A 2.211(7)

Au1A Cl1A 2.278(7)

Au1A Au2A 3.0185(18)

Au2A N1A 2.16(2)

Au2A P3A 2.243(8)

Au2A Au3A 2.9518(18)

Au3A N2A 2.17(2)

Au3A P2A 2.254(8)

Au3A Au4A 2.9688(19)

Au4A P4A 2.222(8)

Au4A Cl2A 2.268(8)

C1A N1A 1.29(3)

C1A C2A 1.38(4)

C1A C6A 1.61(3)

C2A C3A 1.43(4)

C2A H2A 0.9500

C3A C4A 1.42(4)

C3A H3A 0.9500

C4A C5A 1.40(4)

C4A H4A 0.9500

C14A C19A 1.388(5)

C14A C15A 1.389(4)

C14A P1A 1.803(19)

C15A C16A 1.389(4)

C15A H15A 0.9500

C16A C17A 1.389(4)

C16A H16A 0.9500

C17A C18A 1.389(4)

C17A H17A 0.9500

C18A C19A 1.388(4)

C18A H18A 0.9500

C19A H19A 0.9500

C20A C25A 1.389(5)

C20A C21A 1.389(4)

C20A P2A 1.81(3)

C21A C22A 1.390(4)

C21A H21A 0.9500
C22A C23A 1.390(4)
C22A H22A 0.9500
C23A C24A 1.388(4)
C23A H23A 0.9500
C24A C25A 1.390(4)
C24A H24A 0.9500
C25A H25A 0.9500
C20' C25' 1.389(5)
C20' C21' 1.389(4)
C20' P2A 1.95(3)
C21' C22' 1.390(4)
C21' H21' 0.9500
C22' C23' 1.390(4)
C22' H22' 0.9500
C23' C24' 1.390(4)
C23' H23' 0.9500
C24' C25' 1.390(4)
C24' H24' 0.9500
C25' H25' 0.9500
C26A C27A 1.3900
C26A C31A 1.3900
C26A P2A 1.81(2)
C27A C28A 1.3900
C27A H27A 0.9500
C28A C29A 1.3900
C28A H28A 0.9500
C29A C30A 1.3900
C29A H29A 0.9500
C30A C31A 1.3900
C30A H30A 0.9500
C31A H31A 0.9500
N2A C32A 1.26(3)
N2A C36A 1.34(3)
C32A C33A 1.42(4)
C32A C37A 1.495(10)
C33A C34A 1.36(4)
C33A H33A 0.9500
C34A C35A 1.32(3)

C34A H34A 0.9500
C35A C36A 1.46(4)
C35A H35A 0.9500
C36A C38A 1.42(4)
C37A P3A 1.84(3)
C37A H37A 0.9900
C37A H37B 0.9900
C38A P4A 1.86(3)
C38A H38A 0.9900
C38A H38B 0.9900
C39A C44A 1.388(5)
C39A C40A 1.389(4)
C39A P3A 1.801(19)
C40A C41A 1.389(4)
C40A H40A 0.9500
C41A C42A 1.389(4)
C41A H41A 0.9500
C42A C43A 1.389(4)
C42A H42A 0.9500
C43A C44A 1.389(4)
C43A H43A 0.9500
C44A H44A 0.9500
C46A C45A 1.39(3)
C46A C47A 1.46(3)
C46A H46A 0.9500
C47A C48A 1.41(4)
C47A H47A 0.9500
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C48A H48A 0.9500
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C49A H49A 0.9500
C50A C45A 1.44(3)
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C51A C56A 1.3900
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C53A H53A 0.9500
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C58A C59A 1.3900
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C60A H60A 0.9500
C62A C63A 1.3900
C62A H62A 0.9500
C63A H63A 0.9500
N1A C5A 1.41(3)
Au1B P1B 2.250(7)
Au1B Cl1B 2.279(7)
Au1B Au2B 3.0132(18)
Au2B N1B 2.12(2)
Au2B P3B 2.237(9)
Au2B Au3B 2.9813(18)
Au3B N2B 2.175(18)
Au3B P2B 2.261(8)
Au3B Au4B 2.9605(18)
Au4B P4B 2.230(8)
Au4B Cl2B 2.289(7)
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C3B C2B 1.27(4)
C3B H3B 0.9500
C2B C1B 1.30(4)
C2B H2B 0.9500
C1B N1B 1.46(3)
C1B C6B 1.47(4)

C8B C13B 1.388(5)
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C9B C10B 1.389(4)
C9B H9B 0.9500
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C17B H17B 0.9500
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C54B H54B 0.9500
C55B C56B 1.388(4)
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C56B H56B 0.9500
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C60B H60B 0.9500
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C61B H61B 0.9500

C62B H62B 0.9500
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N2B C36B 1.30(3)
N2B C32B 1.33(3)
P1A C6A 1.78(3)
P1A C8A 1.825(15)
P2A C7A 1.85(3)
P3A C45A 1.82(3)
C5A C7A 1.46(4)
C6A H6AA 0.9900
C6A H6AB 0.9900
C7A H7AA 0.9900
C7A H7AB 0.9900
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C10A H10A 0.9500
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C11A H11A 0.9500
C12A C13A 1.3900
C12A H12A 0.9500
C13A H13A 0.9500
P1B C6B 1.89(3)
P2B C20B 1.77(2)
P2B C26B 1.81(2)
P2B C7B 1.85(3)
P3B C37B 1.82(3)
P4B C38B 1.84(3)
C5B C7B 1.50(4)
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C7B H7BA 0.9900
C7B H7BB 0.9900
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C37B H37D 0.9900

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C38B H38D 0.9900
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C23B H23B 0.9500
C24B C25B 1.3900
C24B H24B 0.9500
C25B H25B 0.9500
C26B C27B 1.3900
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C29B H29B 0.9500
C30B C31B 1.3900
C30B H30B 0.9500
C31B H31B 0.9500
Sb1C F1C 1.836(16)
Sb1C F4C 1.869(18)
Sb1C F3C 1.869(18)
Sb1C F6C 1.875(14)
Sb1C F5C 1.880(16)
Sb1C F2C 1.895(17)
Sb1D F6D 1.828(19)
Sb1D F2D 1.85(2)
Sb1D F3D 1.865(19)
Sb1D F1D 1.873(18)
Sb1D F4D 1.893(18)
Sb1D F5D 1.921(19)
Sb1E F4E 1.82(4)
Sb1E F2E 1.82(4)
Sb1E F1E 1.84(3)

Sb1E F3E 1.85(4)
Sb1E F5E 1.86(4)
Sb1E F6E 2.01(5)
Sb2E F5E' 1.80(3)
Sb2E F6E' 1.82(5)
Sb2E F1E' 1.83(3)
Sb2E F2E' 1.85(4)
Sb2E F3E' 1.86(4)
Sb2E F4E' 1.93(3)
Sb1F F2F 1.840(17)
Sb1F F4F 1.857(16)
Sb1F F1F 1.858(14)
Sb1F F6F 1.860(16)
Sb1F F5F 1.869(16)
Sb1F F3F 1.889(16)
Sb2F F2F' 1.836(18)
Sb2F F4F' 1.856(18)
Sb2F F1F' 1.858(16)
Sb2F F6F' 1.862(17)
Sb2F F5F' 1.872(17)
Sb2F F3F' 1.893(18)

Angles----------
P1A Au1A Cl1A 173.4(3)
P1A Au1A Au2A 86.0(2)
Cl1A Au1A Au2A 99.60(19)
N1A Au2A P3A 167.8(6)
N1A Au2A Au3A 79.0(6)
P3A Au2A Au3A 89.8(2)
N1A Au2A Au1A 84.0(6)
P3A Au2A Au1A 106.9(2)
Au3A Au2A Au1A 162.86(6)
N2A Au3A P2A 167.5(7)
N2A Au3A Au2A 78.9(6)
P2A Au3A Au2A 88.6(3)
N2A Au3A Au4A 86.2(6)
P2A Au3A Au4A 106.2(3)
Au2A Au3A Au4A 160.88(5)
P4A Au4A Cl2A 176.5(4)

P4A Au4A Au3A 88.0(2)
Cl2A Au4A Au3A 92.8(3)
N1A C1A C2A 123(3)
N1A C1A C6A 124(2)
C2A C1A C6A 113(2)
C1A C2A C3A 116(3)
C1A C2A H2A 121.9
C3A C2A H2A 121.9
C4A C3A C2A 122(3)
C4A C3A H3A 119.2
C2A C3A H3A 119.2
C5A C4A C3A 118(3)
C5A C4A H4A 121.1
C3A C4A H4A 121.1
C19A C14A C15A 118.9(14)
C19A C14A P1A 118.8(13)
C15A C14A P1A 122.0(13)
C16A C15A C14A 120.9(15)
C16A C15A H15A 119.6
C14A C15A H15A 119.6
C15A C16A C17A 120.2(16)
C15A C16A H16A 119.9
C17A C16A H16A 119.9
C18A C17A C16A 118.6(15)
C18A C17A H17A 120.7
C16A C17A H17A 120.7
C19A C18A C17A 121.2(15)
C19A C18A H18A 119.4
C17A C18A H18A 119.4
C14A C19A C18A 119.9(15)
C14A C19A H19A 120.1
C18A C19A H19A 120.1
C25A C20A C21A 119.0(17)
C25A C20A P2A 118.4(18)
C21A C20A P2A 120.4(19)
C20A C21A C22A 120.7(17)
C20A C21A H21A 119.6
C22A C21A H21A 119.6
C23A C22A C21A 117.1(17)

C23A C22A H22A 121.5
C21A C22A H22A 121.5
C24A C23A C22A 116.6(18)
C24A C23A H23A 121.7
C22A C23A H23A 121.7
C23A C24A C25A 119.5(17)
C23A C24A H24A 120.2
C25A C24A H24A 120.2
C20A C25A C24A 117.8(16)
C20A C25A H25A 121.1
C24A C25A H25A 121.1
C25' C20' C21' 119.8(18)
C25' C20' P2A 122(3)
C21' C20' P2A 118(3)
C20' C21' C22' 119.2(18)
C20' C21' H21' 120.4
C22' C21' H21' 120.4
C21' C22' C23' 117(2)
C21' C22' H22' 121.4
C23' C22' H22' 121.4
C24' C23' C22' 117(2)
C24' C23' H23' 121.3
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C23' C24' C25' 117(2)
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C24' C25' H25' 120.1
C27A C26A C31A 120.0
C27A C26A P2A 118.2(18)
C31A C26A P2A 121.6(17)
C26A C27A C28A 120.0
C26A C27A H27A 120.0
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C29A C28A H28A 120.0
C27A C28A H28A 120.0
C28A C29A C30A 120.0

C28A C29A H29A 120.0
C30A C29A H29A 120.0
C29A C30A C31A 120.0
C29A C30A H30A 120.0
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C26A C31A H31A 120.0
C32A N2A C36A 123(2)
C32A N2A Au3A 119.1(17)
C36A N2A Au3A 118.0(19)
N2A C32A C33A 124(2)
N2A C32A C37A 120(2)
C33A C32A C37A 115(2)
C34A C33A C32A 114(3)
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C32A C33A H33A 123.1
C35A C34A C33A 125(3)
C35A C34A H34A 117.5
C33A C34A H34A 117.5
C34A C35A C36A 118(3)
C34A C35A H35A 121.2
C36A C35A H35A 121.2
N2A C36A C38A 122(3)
N2A C36A C35A 117(3)
C38A C36A C35A 121(3)
C32A C37A P3A 114(2)
C32A C37A H37A 108.7
P3A C37A H37A 108.7
C32A C37A H37B 108.7
P3A C37A H37B 108.7
H37A C37A H37B 107.6
C36A C38A P4A 112(2)
C36A C38A H38A 109.2
P4A C38A H38A 109.2
C36A C38A H38B 109.2
P4A C38A H38B 109.2
H38A C38A H38B 107.9
C44A C39A C40A 120.2(15)

C44A C39A P3A 122.5(14)
C40A C39A P3A 117.3(15)
C41A C40A C39A 119.8(16)
C41A C40A H40A 120.1
C39A C40A H40A 120.1
C40A C41A C42A 120.2(16)
C40A C41A H41A 119.9
C42A C41A H41A 119.9
C43A C42A C41A 119.6(15)
C43A C42A H42A 120.2
C41A C42A H42A 120.2
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C42A C43A H43A 119.8
C44A C43A H43A 119.8
C39A C44A C43A 119.5(15)
C39A C44A H44A 120.2
C43A C44A H44A 120.2
C45A C46A C47A 115(2)
C45A C46A H46A 122.3
C47A C46A H46A 122.3
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C52A C51A C56A 120.0
C52A C51A P4A 122.0(15)
C56A C51A P4A 118.0(15)
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C53A C52A H52A 120.0
C54A C53A C52A 120.0

C54A C53A H53A 120.0
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C63A C57A P4A 118.0(15)
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C59A C58A H58A 120.0
C57A C58A H58A 120.0
C60A C59A C58A 120.0
C60A C59A H59A 120.0
C58A C59A H59A 120.0
C59A C60A C62A 120.0
C59A C60A H60A 120.0
C62A C60A H60A 120.0
C63A C62A C60A 120.0
C63A C62A H62A 120.0
C60A C62A H62A 120.0
C62A C63A C57A 120.0
C62A C63A H63A 120.0
C57A C63A H63A 120.0
C1A N1A C5A 124(2)
C1A N1A Au2A 117.0(18)
C5A N1A Au2A 118.4(15)
P1B Au1B Cl1B 174.3(3)
P1B Au1B Au2B 88.2(2)
Cl1B Au1B Au2B 97.07(19)
N1B Au2B P3B 166.5(7)
N1B Au2B Au3B 77.8(6)
P3B Au2B Au3B 89.4(2)
N1B Au2B Au1B 83.1(6)

P3B Au2B Au1B 109.6(2)
Au3B Au2B Au1B 160.97(6)
N2B Au3B P2B 167.2(6)
N2B Au3B Au4B 84.2(5)
P2B Au3B Au4B 108.4(3)
N2B Au3B Au2B 78.3(5)
P2B Au3B Au2B 88.9(3)
Au4B Au3B Au2B 158.63(5)
P4B Au4B Cl2B 176.9(3)
P4B Au4B Au3B 88.6(2)
Cl2B Au4B Au3B 90.8(2)
C5B C4B C3B 121(3)
C5B C4B H4B 119.3
C3B C4B H4B 119.3
C2B C3B C4B 115(3)
C2B C3B H3B 122.3
C4B C3B H3B 122.3
C3B C2B C1B 127(3)
C3B C2B H2B 116.7
C1B C2B H2B 116.7
C2B C1B N1B 118(3)
C2B C1B C6B 131(3)
N1B C1B C6B 111(2)
C13B C8B C9B 120.5(15)
C13B C8B P1B 120.3(13)
C9B C8B P1B 119.2(13)
C10B C9B C8B 119.0(15)
C10B C9B H9B 120.5
C8B C9B H9B 120.5
C11B C10B C9B 119.1(15)
C11B C10B H10B 120.4
C9B C10B H10B 120.4
C12B C11B C10B 123.0(15)
C12B C11B H11B 118.5
C10B C11B H11B 118.5
C11B C12B C13B 116.6(14)
C11B C12B H12B 121.7
C13B C12B H12B 121.7
C8B C13B C12B 121.5(14)

C8B C13B H13B 119.2
C12B C13B H13B 119.2
C19B C14B C15B 120.0
C19B C14B P1B 120.1(11)
C15B C14B P1B 119.8(11)
C14B C19B C18B 120.0
C14B C19B H19B 120.0
C18B C19B H19B 120.0
C17B C18B C19B 120.0
C17B C18B H18B 120.0
C19B C18B H18B 120.0
C16B C17B C18B 120.0
C16B C17B H17B 120.0
C18B C17B H17B 120.0
C17B C16B C15B 120.0
C17B C16B H16B 120.0
C15B C16B H16B 120.0
C16B C15B C14B 120.0
C16B C15B H15B 120.0
C14B C15B H15B 120.0
C32B C33B C34B 116(3)
C32B C33B H33B 122.2
C34B C33B H33B 122.2
C35B C34B C33B 118(3)
C35B C34B H34B 121.0
C33B C34B H34B 121.0
C36B C35B C34B 122(3)
C36B C35B H35B 119.1
C34B C35B H35B 119.1
C44B C39B C40B 119.2(15)
C44B C39B P3B 122.0(15)
C40B C39B P3B 118.0(15)
C39B C40B C41B 119.5(16)
C39B C40B H40B 120.2
C41B C40B H40B 120.2
C42B C41B C40B 119.5(17)
C42B C41B H41B 120.2
C40B C41B H41B 120.2
C43B C42B C41B 119.0(16)

C43B C42B H42B 120.5
C41B C42B H42B 120.5
C44B C43B C42B 119.8(15)
C44B C43B H43B 120.1
C42B C43B H43B 120.1
C39B C44B C43B 120.0(15)
C39B C44B H44B 120.0
C43B C44B H44B 120.0
C50B C45B C46B 120.3(14)
C50B C45B P3B 118.6(13)
C46B C45B P3B 121.1(13)
C45B C46B C47B 120.4(15)
C45B C46B H46B 119.8
C47B C46B H46B 119.8
C46B C47B C48B 118.5(16)
C46B C47B H47B 120.7
C48B C47B H47B 120.7
C47B C48B C49B 122.0(16)
C47B C48B H48B 119.0
C49B C48B H48B 119.0
C48B C49B C50B 118.6(15)
C48B C49B H49B 120.7
C50B C49B H49B 120.7
C45B C50B C49B 120.2(14)
C45B C50B H50B 119.9
C49B C50B H50B 119.9
C56B C51B C52B 121.3(16)
C56B C51B P4B 115.7(16)
C52B C51B P4B 123.0(16)
C51B C52B C53B 118.7(16)
C51B C52B H52B 120.6
C53B C52B H52B 120.6
C54B C53B C52B 119.8(16)
C54B C53B H53B 120.1
C52B C53B H53B 120.1
C53B C54B C55B 120.8(16)
C53B C54B H54B 119.6
C55B C54B H54B 119.6
C56B C55B C54B 118.9(16)

C56B C55B H55B 120.6
C54B C55B H55B 120.6
C55B C56B C51B 118.7(16)
C55B C56B H56B 120.7
C51B C56B H56B 120.7
C62B C57B C58B 118.3(15)
C62B C57B P4B 118.2(14)
C58B C57B P4B 123.6(14)
C59B C58B C57B 120.4(15)
C59B C58B H58B 119.8
C57B C58B H58B 119.8
C60B C59B C58B 120.3(16)
C60B C59B H59B 119.9
C58B C59B H59B 119.9
C59B C60B C61B 119.7(16)
C59B C60B H60B 120.1
C61B C60B H60B 120.1
C62B C61B C60B 118.6(15)
C62B C61B H61B 120.7
C60B C61B H61B 120.7
C57B C62B C61B 121.9(15)
C57B C62B H62B 119.0
C61B C62B H62B 119.0
C5B N1B C1B 118(2)
C5B N1B Au2B 121.0(17)
C1B N1B Au2B 120.0(17)
C36B N2B C32B 122(2)
C36B N2B Au3B 120.2(17)
C32B N2B Au3B 118.2(16)
C6A P1A C14A 104.3(12)
C6A P1A C8A 100.2(10)
C14A P1A C8A 105.9(9)
C6A P1A Au1A 118.4(8)
C14A P1A Au1A 111.0(7)
C8A P1A Au1A 115.5(7)
C20A P2A C26A 106.4(18)
C20A P2A C7A 108.7(14)
C26A P2A C7A 106.0(14)
C26A P2A C20' 106.4(17)

C7A P2A C20' 99(2)
C20A P2A Au3A 110.1(12)
C26A P2A Au3A 117.1(11)
C7A P2A Au3A 108.2(10)
C20' P2A Au3A 118(2)
C39A P3A C45A 106.3(12)
C39A P3A C37A 107.7(10)
C45A P3A C37A 102.4(12)
C39A P3A Au2A 116.9(8)
C45A P3A Au2A 114.3(9)
C37A P3A Au2A 108.1(9)
C57A P4A C51A 110.1(12)
C57A P4A C38A 101.3(13)
C51A P4A C38A 106.1(13)
C57A P4A Au4A 113.7(9)
C51A P4A Au4A 111.7(9)
C38A P4A Au4A 113.1(9)
C4A C5A N1A 117(2)
C4A C5A C7A 125(3)
N1A C5A C7A 118(2)
C1A C6A P1A 109.2(17)
C1A C6A H6AA 109.9
P1A C6A H6AA 109.9
C1A C6A H6AB 109.9
P1A C6A H6AB 109.9
H6AA C6A H6AB 108.3
C5A C7A P2A 112(2)
C5A C7A H7AA 109.2
P2A C7A H7AA 109.2
C5A C7A H7AB 109.2
P2A C7A H7AB 109.2
H7AA C7A H7AB 107.9
C9A C8A C13A 120.0
C9A C8A P1A 123.4(11)
C13A C8A P1A 116.4(11)
C8A C9A C10A 120.0
C8A C9A H9A 120.0
C10A C9A H9A 120.0
C11A C10A C9A 120.0

C11A C10A H10A 120.0
C9A C10A H10A 120.0
C10A C11A C12A 120.0
C10A C11A H11A 120.0
C12A C11A H11A 120.0
C11A C12A C13A 120.0
C11A C12A H12A 120.0
C13A C12A H12A 120.0
C12A C13A C8A 120.0
C12A C13A H13A 120.0
C8A C13A H13A 120.0
C46A C45A C50A 122(2)
C46A C45A P3A 119.1(19)
C50A C45A P3A 117.7(19)
C8B P1B C14B 107.8(10)
C8B P1B C6B 107.5(14)
C14B P1B C6B 107.4(12)
C8B P1B Au1B 108.5(8)
C14B P1B Au1B 115.9(8)
C6B P1B Au1B 109.4(10)
C20B P2B C26B 106.9(16)
C20B P2B C7B 97.8(15)
C26B P2B C7B 104.9(15)
C20B P2B Au3B 123.4(12)
C26B P2B Au3B 114.2(12)
C7B P2B Au3B 107.0(10)
C37B P3B C39B 105.7(12)
C37B P3B C45B 101.0(12)
C39B P3B C45B 109.0(12)
C37B P3B Au2B 109.1(9)
C39B P3B Au2B 115.9(8)
C45B P3B Au2B 114.7(7)
C51B P4B C57B 108.5(14)
C51B P4B C38B 104.8(13)
C57B P4B C38B 102.1(13)
C51B P4B Au4B 113.0(9)
C57B P4B Au4B 115.5(7)
C38B P4B Au4B 111.9(9)
N1B C5B C4B 120(3)

N1B C5B C7B 122(2)
C4B C5B C7B 118(3)
C1B C6B P1B 116(2)
C1B C6B H6BA 108.4
P1B C6B H6BA 108.4
C1B C6B H6BB 108.4
P1B C6B H6BB 108.4
H6BA C6B H6BB 107.4
C5B C7B P2B 110(2)
C5B C7B H7BA 109.6
P2B C7B H7BA 109.6
C5B C7B H7BB 109.6
P2B C7B H7BB 109.6
H7BA C7B H7BB 108.1
N2B C32B C33B 123(2)
N2B C32B C37B 119(2)
C33B C32B C37B 118(2)
N2B C36B C35B 120(3)
N2B C36B C38B 121(2)
C35B C36B C38B 119(3)
C32B C37B P3B 112(2)
C32B C37B H37C 109.2
P3B C37B H37C 109.2
C32B C37B H37D 109.2
P3B C37B H37D 109.2
H37C C37B H37D 107.9
C36B C38B P4B 114(2)
C36B C38B H38C 108.7
P4B C38B H38C 108.7
C36B C38B H38D 108.7
P4B C38B H38D 108.7
H38C C38B H38D 107.6
C21B C20B C25B 120.0
C21B C20B P2B 119(2)
C25B C20B P2B 121(2)
C22B C21B C20B 120.0
C22B C21B H21B 120.0
C20B C21B H21B 120.0
C21B C22B C23B 120.0

C21B C22B H22B 120.0
C23B C22B H22B 120.0
C24B C23B C22B 120.0
C24B C23B H23B 120.0
C22B C23B H23B 120.0
C23B C24B C25B 120.0
C23B C24B H24B 120.0
C25B C24B H24B 120.0
C24B C25B C20B 120.0
C24B C25B H25B 120.0
C20B C25B H25B 120.0
C27B C26B C31B 120.0
C27B C26B P2B 120(2)
C31B C26B P2B 119(2)
C26B C27B C28B 120.0
C26B C27B H27B 120.0
C28B C27B H27B 120.0
C29B C28B C27B 120.0
C29B C28B H28B 120.0
C27B C28B H28B 120.0
C28B C29B C30B 120.0
C28B C29B H29B 120.0
C30B C29B H29B 120.0
C31B C30B C29B 120.0
C31B C30B H30B 120.0
C29B C30B H30B 120.0
C30B C31B C26B 120.0
C30B C31B H31B 120.0
C26B C31B H31B 120.0
F1C Sb1C F4C 90.6(8)
F1C Sb1C F3C 86.7(8)
F4C Sb1C F3C 89.1(8)
F1C Sb1C F6C 179.7(8)
F4C Sb1C F6C 89.1(8)
F3C Sb1C F6C 93.2(7)
F1C Sb1C F5C 88.9(8)
F4C Sb1C F5C 90.1(8)
F3C Sb1C F5C 175.5(8)
F6C Sb1C F5C 91.2(7)

F1C Sb1C F2C 89.8(8)
F4C Sb1C F2C 178.9(9)
F3C Sb1C F2C 89.9(8)
F6C Sb1C F2C 90.5(7)
F5C Sb1C F2C 90.9(8)
F6D Sb1D F2D 93.2(11)
F6D Sb1D F3D 88.6(9)
F2D Sb1D F3D 92.0(9)
F6D Sb1D F1D 177.3(9)
F2D Sb1D F1D 88.7(9)
F3D Sb1D F1D 93.2(9)
F6D Sb1D F4D 89.3(9)
F2D Sb1D F4D 177.3(9)
F3D Sb1D F4D 89.0(8)
F1D Sb1D F4D 88.7(8)
F6D Sb1D F5D 90.9(9)
F2D Sb1D F5D 91.9(10)
F3D Sb1D F5D 176.1(9)
F1D Sb1D F5D 87.2(8)
F4D Sb1D F5D 87.1(8)
F4E Sb1E F2E 172(2)
F4E Sb1E F1E 87.2(17)
F2E Sb1E F1E 89.2(16)
F4E Sb1E F3E 86.5(17)
F2E Sb1E F3E 86.7(17)
F1E Sb1E F3E 93.3(17)
F4E Sb1E F5E 94.0(18)
F2E Sb1E F5E 92.9(18)
F1E Sb1E F5E 88.1(17)
F3E Sb1E F5E 178.5(17)
F4E Sb1E F6E 93(2)
F2E Sb1E F6E 91(2)
F1E Sb1E F6E 174(2)
F3E Sb1E F6E 93(2)
F5E Sb1E F6E 86(2)
F5E' Sb2E F6E' 95(2)
F5E' Sb2E F1E' 90.9(14)
F6E' Sb2E F1E' 172(2)
F5E' Sb2E F2E' 91.1(17)

F6E' Sb2E F2E' 87(2)
F1E' Sb2E F2E' 88.2(14)
F5E' Sb2E F3E' 175.9(18)
F6E' Sb2E F3E' 86(2)
F1E' Sb2E F3E' 88.2(16)
F2E' Sb2E F3E' 84.9(19)
F5E' Sb2E F4E' 90.9(16)
F6E' Sb2E F4E' 94(2)
F1E' Sb2E F4E' 91.2(13)
F2E' Sb2E F4E' 177.9(17)
F3E' Sb2E F4E' 93.1(17)
F2F Sb1F F4F 177.9(16)
F2F Sb1F F1F 92.5(14)
F4F Sb1F F1F 86.7(13)
F2F Sb1F F6F 91.3(13)
F4F Sb1F F6F 89.5(13)
F1F Sb1F F6F 176.1(14)
F2F Sb1F F5F 89.5(14)
F4F Sb1F F5F 92.5(15)
F1F Sb1F F5F 92.1(12)
F6F Sb1F F5F 88.7(12)
F2F Sb1F F3F 85.5(14)
F4F Sb1F F3F 92.6(14)
F1F Sb1F F3F 87.8(12)
F6F Sb1F F3F 91.7(12)
F5F Sb1F F3F 174.9(15)
F2F' Sb2F F4F' 178.7(14)
F2F' Sb2F F1F' 94.1(14)
F4F' Sb2F F1F' 87.2(12)
F2F' Sb2F F6F' 91.6(14)
F4F' Sb2F F6F' 87.1(13)
F1F' Sb2F F6F' 174.1(14)
F2F' Sb2F F5F' 88.9(14)
F4F' Sb2F F5F' 91.0(14)
F1F' Sb2F F5F' 91.8(12)
F6F' Sb2F F5F' 89.8(13)
F2F' Sb2F F3F' 85.7(14)
F4F' Sb2F F3F' 94.4(12)
F1F' Sb2F F3F' 86.9(12)

F6F' Sb2F F3F' 91.9(13)

F5F' Sb2F F3F' 174.4(15)

Table 3. Torsion angles [°] for **Complex 3**.

N1A C1A C2A C3A 1(5)

C6A C1A C2A C3A -178(3)

C1A C2A C3A C4A -5(5)

C2A C3A C4A C5A 6(5)

C19A C14A C15A C16A 5(5)

P1A C14A C15A C16A 179(2)

C14A C15A C16A C17A -1(5)

C15A C16A C17A C18A -3(5)

C16A C17A C18A C19A 3(5)

C15A C14A C19A C18A -5(4)

P1A C14A C19A C18A -179(2)

C17A C18A C19A C14A 1(5)

C25A C20A C21A C22A 14(7)

P2A C20A C21A C22A 177(3)

C20A C21A C22A C23A 6(6)

C21A C22A C23A C24A -30(5)

C22A C23A C24A C25A 34(5)

C21A C20A C25A C24A -10(6)

P2A C20A C25A C24A -174(3)

C23A C24A C25A C20A -13(6)

C25' C20' C21' C22' -4(11)

P2A C20' C21' C22' 172(5)

C20' C21' C22' C23' -16(10)

C21' C22' C23' C24' 35(8)

C22' C23' C24' C25' -34(8)

C21' C20' C25' C24' 5(12)

P2A C20' C25' C24' -170(6)

C23' C24' C25' C20' 13(10)

C31A C26A C27A C28A 0.0

P2A C26A C27A C28A -175(2)

C26A C27A C28A C29A 0.0

C27A C28A C29A C30A 0.0

C28A C29A C30A C31A 0.0

C29A C30A C31A C26A 0.0

C27A C26A C31A C30A 0.0

P2A C26A C31A C30A 175(2)

C36A N2A C32A C33A -6(5)

Au3A N2A C32A C33A 178(2)

C36A N2A C32A C37A -172(3)

Au3A N2A C32A C37A 12(4)

N2A C32A C33A C34A 7(5)

C37A C32A C33A C34A 174(3)

C32A C33A C34A C35A -7(5)

C33A C34A C35A C36A 5(4)

C32A N2A C36A C38A 174(3)

Au3A N2A C36A C38A -10(4)

C32A N2A C36A C35A 3(4)

Au3A N2A C36A C35A 179.2(19)

C34A C35A C36A N2A -2(4)

C34A C35A C36A C38A -174(3)

N2A C32A C37A P3A 76(3)

C33A C32A C37A P3A -91(3)

N2A C36A C38A P4A 86(3)

C35A C36A C38A P4A -103(3)

C44A C39A C40A C41A -6(5)

P3A C39A C40A C41A 176(3)

C39A C40A C41A C42A 3(6)

C40A C41A C42A C43A 1(5)

C41A C42A C43A C44A -1(5)

C40A C39A C44A C43A 6(4)

P3A C39A C44A C43A -176(2)

C42A C43A C44A C39A -2(4)

C45A C46A C47A C48A 7(4)

C46A C47A C48A C49A -4(4)

C47A C48A C49A C50A 1(4)

C48A C49A C50A C45A -3(4)

C56A C51A C52A C53A 0.0

P4A C51A C52A C53A 177.7(17)

C51A C52A C53A C54A 0.0

C52A C53A C54A C55A 0.0

C53A C54A C55A C56A 0.0

C54A C55A C56A C51A 0.0

C52A C51A C56A C55A 0.0

P4A C51A C56A C55A -177.8(17)

C63A C57A C58A C59A 0.0

P4A C57A C58A C59A 174.5(18)

C57A C58A C59A C60A 0.0

C58A C59A C60A C62A 0.0

C59A C60A C62A C63A 0.0

C60A C62A C63A C57A 0.0

C58A C57A C63A C62A 0.0

P4A C57A C63A C62A -174.7(17)

C2A C1A N1A C5A 2(4)

C6A C1A N1A C5A -179(2)

C2A C1A N1A Au2A -171(2)

C6A C1A N1A Au2A 8(3)

C5B C4B C3B C2B 5(5)

C4B C3B C2B C1B -4(5)

C3B C2B C1B N1B 2(5)

C3B C2B C1B C6B 178(4)

C13B C8B C9B C10B 0(5)

P1B C8B C9B C10B -179(2)

C8B C9B C10B C11B -2(5)

C9B C10B C11B C12B 0(5)

C10B C11B C12B C13B 4(5)

C9B C8B C13B C12B 4(4)

P1B C8B C13B C12B -177(2)

C11B C12B C13B C8B -6(4)

C15B C14B C19B C18B 0.0

P1B C14B C19B C18B 177.6(15)

C14B C19B C18B C17B 0.0

C19B C18B C17B C16B 0.0

C18B C17B C16B C15B 0.0

C17B C16B C15B C14B 0.0

C19B C14B C15B C16B 0.0

P1B C14B C15B C16B -177.6(15)

C32B C33B C34B C35B -1(4)

C33B C34B C35B C36B -1(4)

C44B C39B C40B C41B 5(5)

P3B C39B C40B C41B -165(3)

C39B C40B C41B C42B -17(6)
C40B C41B C42B C43B 16(5)
C41B C42B C43B C44B -2(5)
C40B C39B C44B C43B 9(4)
P3B C39B C44B C43B 179(2)
C42B C43B C44B C39B -10(4)
C50B C45B C46B C47B -2(5)
P3B C45B C46B C47B 177(3)
C45B C46B C47B C48B 1(5)
C46B C47B C48B C49B -1(6)
C47B C48B C49B C50B 2(5)
C46B C45B C50B C49B 3(4)
P3B C45B C50B C49B -176(2)
C48B C49B C50B C45B -3(5)
C56B C51B C52B C53B 6(5)
P4B C51B C52B C53B -176(3)
C51B C52B C53B C54B -1(5)
C52B C53B C54B C55B 3(6)
C53B C54B C55B C56B -10(6)
C54B C55B C56B C51B 16(5)
C52B C51B C56B C55B -14(5)
P4B C51B C56B C55B 168(3)
C62B C57B C58B C59B -3(5)
P4B C57B C58B C59B 177(2)
C57B C58B C59B C60B 4(5)
C58B C59B C60B C61B -8(5)
C59B C60B C61B C62B 10(5)
C58B C57B C62B C61B 5(5)
P4B C57B C62B C61B -175(2)
C60B C61B C62B C57B -9(5)
C2B C1B N1B C5B -2(4)
C6B C1B N1B C5B -178(3)
C2B C1B N1B Au2B 166(2)
C6B C1B N1B Au2B -10(3)
C19A C14A P1A C6A -88(2)
C15A C14A P1A C6A 99(2)
C19A C14A P1A C8A 167(2)
C15A C14A P1A C8A -6(3)
C19A C14A P1A Au1A 41(2)

C15A C14A P1A Au1A -132(2)
C25A C20A P2A C26A -100(4)
C21A C20A P2A C26A 97(4)
C25A C20A P2A C7A 147(3)
C21A C20A P2A C7A -16(4)
C25A C20A P2A Au3A 28(4)
C21A C20A P2A Au3A -135(3)
C27A C26A P2A C20A -34.4(19)
C31A C26A P2A C20A 150.3(17)
C27A C26A P2A C7A 81.2(18)
C31A C26A P2A C7A -94.2(19)
C27A C26A P2A C20' -24(3)
C31A C26A P2A C20' 161(3)
C27A C26A P2A Au3A -157.9(12)
C31A C26A P2A Au3A 27(2)
C44A C39A P3A C45A 88(3)
C40A C39A P3A C45A -94(3)
C44A C39A P3A C37A -21(3)
C40A C39A P3A C37A 157(2)
C44A C39A P3A Au2A -143(2)
C40A C39A P3A Au2A 35(3)
C32A C37A P3A C39A -179(2)
C32A C37A P3A C45A 69(2)
C32A C37A P3A Au2A -52(2)
C58A C57A P4A C51A 141.2(14)
C63A C57A P4A C51A -44.2(16)
C58A C57A P4A C38A -106.8(15)
C63A C57A P4A C38A 67.8(15)
C58A C57A P4A Au4A 14.9(16)
C63A C57A P4A Au4A -170.5(10)
C52A C51A P4A C57A 98.1(16)
C56A C51A P4A C57A -84.2(15)
C52A C51A P4A C38A -10.8(17)
C56A C51A P4A C38A 166.9(14)
C52A C51A P4A Au4A -134.5(12)
C56A C51A P4A Au4A 43.2(14)
C36A C38A P4A C57A 71(2)
C36A C38A P4A C51A -174(2)
C36A C38A P4A Au4A -51(2)

C3A C4A C5A N1A -3(4)
C3A C4A C5A C7A 173(3)
C1A N1A C5A C4A -1(4)
Au2A N1A C5A C4A 172(2)
C1A N1A C5A C7A -178(3)
Au2A N1A C5A C7A -5(3)
N1A C1A C6A P1A 73(3)
C2A C1A C6A P1A -108(2)
C14A P1A C6A C1A 71.5(18)
C8A P1A C6A C1A -179.0(16)
Au1A P1A C6A C1A -52.5(19)
C4A C5A C7A P2A -91(3)
N1A C5A C7A P2A 85(3)
C20A P2A C7A C5A -167(2)
C26A P2A C7A C5A 79(2)
C20' P2A C7A C5A -171(3)
Au3A P2A C7A C5A -47(2)
C6A P1A C8A C9A -24.3(16)
C14A P1A C8A C9A 83.9(15)
Au1A P1A C8A C9A -152.8(10)
C6A P1A C8A C13A 160.9(13)
C14A P1A C8A C13A -90.9(14)
Au1A P1A C8A C13A 32.5(13)
C13A C8A C9A C10A 0.0
P1A C8A C9A C10A -174.6(17)
C8A C9A C10A C11A 0.0
C9A C10A C11A C12A 0.0
C10A C11A C12A C13A 0.0
C11A C12A C13A C8A 0.0
C9A C8A C13A C12A 0.0
P1A C8A C13A C12A 175.0(15)
C47A C46A C45A C50A -8(4)
C47A C46A C45A P3A -175(2)
C49A C50A C45A C46A 6(4)
C49A C50A C45A P3A 174(2)
C39A P3A C45A C46A -32(2)
C37A P3A C45A C46A 80(2)
Au2A P3A C45A C46A -162.9(19)
C39A P3A C45A C50A 160(2)

C37A P3A C45A C50A -87(2)
Au2A P3A C45A C50A 29(2)
C13B C8B P1B C14B -173(2)
C9B C8B P1B C14B 7(3)
C13B C8B P1B C6B 72(3)
C9B C8B P1B C6B -109(3)
C13B C8B P1B Au1B -46(3)
C9B C8B P1B Au1B 133(2)
C19B C14B P1B C8B -79.5(15)
C15B C14B P1B C8B 98.1(15)
C19B C14B P1B C6B 36.1(16)
C15B C14B P1B C6B -146.3(15)
C19B C14B P1B Au1B 158.7(9)
C15B C14B P1B Au1B -23.7(14)
C44B C39B P3B C37B 28(3)
C40B C39B P3B C37B -162(3)
C44B C39B P3B C45B -79(3)
C40B C39B P3B C45B 90(3)
C44B C39B P3B Au2B 149(2)
C40B C39B P3B Au2B -41(3)
C50B C45B P3B C37B 96(2)
C46B C45B P3B C37B -84(2)
C50B C45B P3B C39B -153(2)
C46B C45B P3B C39B 27(3)
C50B C45B P3B Au2B -21(2)
C46B C45B P3B Au2B 159(2)
C56B C51B P4B C57B 98(3)
C52B C51B P4B C57B -80(3)
C56B C51B P4B C38B -154(3)
C52B C51B P4B C38B 29(3)
C56B C51B P4B Au4B -31(3)
C52B C51B P4B Au4B 151(3)
C62B C57B P4B C51B -134(2)
C58B C57B P4B C51B 46(3)
C62B C57B P4B C38B 116(2)
C58B C57B P4B C38B -64(3)
C62B C57B P4B Au4B -5(3)
C58B C57B P4B Au4B 175(2)
C1B N1B C5B C4B 3(4)

Au2B N1B C5B C4B -165(2)
C1B N1B C5B C7B -179(3)
Au2B N1B C5B C7B 13(4)
C3B C4B C5B N1B -5(5)
C3B C4B C5B C7B 177(3)
C2B C1B C6B P1B 104(4)
N1B C1B C6B P1B -81(3)
C8B P1B C6B C1B -55(3)
C14B P1B C6B C1B -171(2)
Au1B P1B C6B C1B 63(2)
N1B C5B C7B P2B -89(3)
C4B C5B C7B P2B 90(3)
C20B P2B C7B C5B -90(2)
C26B P2B C7B C5B 160(2)
Au3B P2B C7B C5B 38(2)
C36B N2B C32B C33B -3(4)
Au3B N2B C32B C33B 178(2)
C36B N2B C32B C37B 171(3)
Au3B N2B C32B C37B -8(3)
C34B C33B C32B N2B 2(4)
C34B C33B C32B C37B -171(3)
C32B N2B C36B C35B 1(4)
Au3B N2B C36B C35B -180(2)
C32B N2B C36B C38B -174(3)
Au3B N2B C36B C38B 5(4)
C34B C35B C36B N2B 1(5)
C34B C35B C36B C38B 176(3)
N2B C32B C37B P3B -80(3)
C33B C32B C37B P3B 94(3)
C39B P3B C37B C32B 178.7(19)
C45B P3B C37B C32B -68(2)
Au2B P3B C37B C32B 53(2)
N2B C36B C38B P4B -82(3)
C35B C36B C38B P4B 103(3)
C51B P4B C38B C36B 171(2)
C57B P4B C38B C36B -76(2)
Au4B P4B C38B C36B 48(2)
C26B P2B C20B C21B -128.3(19)
C7B P2B C20B C21B 123.4(17)

Au3B P2B C20B C21B 7(2)
C26B P2B C20B C25B 49(2)
C7B P2B C20B C25B -59.0(19)
Au3B P2B C20B C25B -175.4(12)
C25B C20B C21B C22B 0.0
P2B C20B C21B C22B 178(2)
C20B C21B C22B C23B 0.0
C21B C22B C23B C24B 0.0
C22B C23B C24B C25B 0.0
C23B C24B C25B C20B 0.0
C21B C20B C25B C24B 0.0
P2B C20B C25B C24B -177(2)
C20B P2B C26B C27B -165.2(19)
C7B P2B C26B C27B -62(2)
Au3B P2B C26B C27B 55(2)
C20B P2B C26B C31B 12(2)
C7B P2B C26B C31B 115(2)
Au3B P2B C26B C31B -128.4(16)
C31B C26B C27B C28B 0.0
P2B C26B C27B C28B 177(3)
C26B C27B C28B C29B 0.0
C27B C28B C29B C30B 0.0
C28B C29B C30B C31B 0.0
C29B C30B C31B C26B 0.0
C27B C26B C31B C30B 0.0
P2B C26B C31B C30B -177(3)

Symetry operations

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1 'x, y, z'
2 '-x, y+1/2, -z+1/2'
3 '-x, -y, -z'
4 'x, -y-1/2, z-1/2'

Complex 5

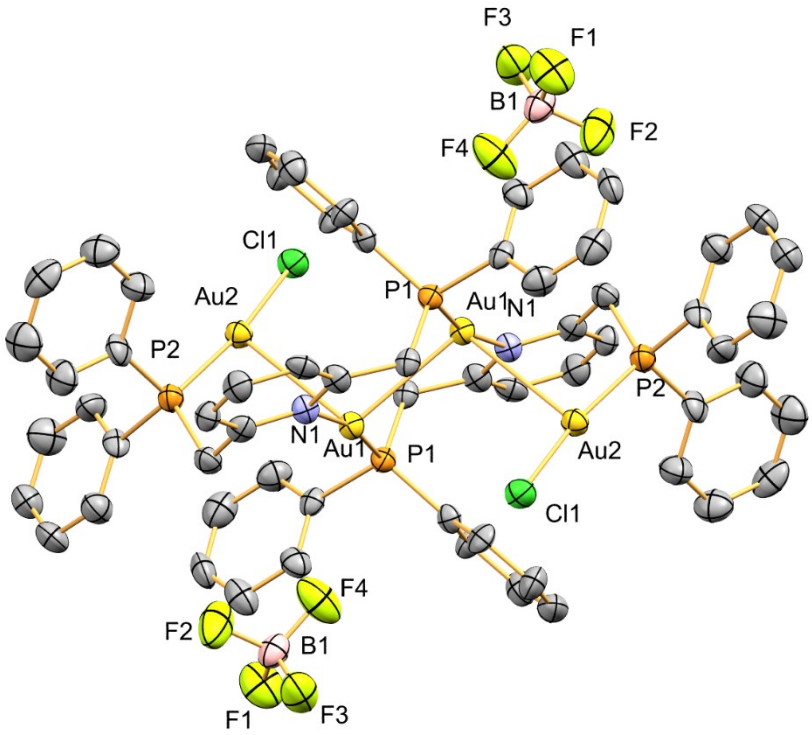
F3
F1
B1
F2
F4
Cl1
Au2
P1
Au1
N1
P2
P2
N1
Au1
P1
Au2
Cl1
F4
F2
B1
F1
F3

Table 1. Crystal data and structure refinement for **Complex 5**.

Identification code	**Complex 5**	
Empirical formula	C66 H60 Au4 B2 Cl2 F8 N4 P4	
Formula weight	2065.44	
Temperature	150.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 15.1241(12) Å	α= 90°.
	b = 10.3724(8) Å	β= 101.162(3)°.
	c = 20.8748(16) Å	γ = 90°.
Volume	3212.8(4) $Å^3$	
Z	2	
Density (calculated)	2.135 Mg/m^3	
Absorption coefficient	9.356 mm^{-1}	
F(000)	1952	
Crystal size	0.17 x 0.06 x 0.04 mm^3	
Theta range for data collection	0.994 to 25.027°.	
Index ranges	-18<=h<=17, -12<=k<=12, 0<=l<=24	
Reflections collected	11200	
Independent reflections	5730 [R(int) = 0.0542]	
Completeness to theta = 25.027°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.046758 and 0.012757	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5730 / 16 / 360	
Goodness-of-fit on F^2	1.126	
Final R indices [I>2sigma(I)]	R1 = 0.0596, wR2 = 0.1272	
R indices (all data)	R1 = 0.0724, wR2 = 0.1329	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.716 and -1.559 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **Complex 5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	5415(1)	5951(1)	4608(1)	29(1)
Au(2)	7514(1)	5142(1)	5208(1)	32(1)
Cl(1)	7486(3)	3080(4)	5609(2)	40(1)
P(1)	4663(3)	5751(4)	6073(2)	28(1)
P(2)	7789(3)	7094(4)	4836(2)	33(1)
N(1)	5627(7)	7748(12)	5096(6)	29(3)
C(1)	3832(6)	5438(10)	6578(5)	30(3)
C(6)	3025(7)	6113(10)	6511(5)	46(4)
C(5)	2411(6)	5807(11)	6904(6)	53(5)
C(4)	2604(7)	4827(12)	7364(5)	47(5)
C(3)	3411(8)	4153(10)	7431(5)	48(5)
C(2)	4025(6)	4458(10)	7038(5)	41(4)
C(7)	5713(5)	5982(9)	6638(4)	29(3)
C(8)	6448(6)	5188(9)	6618(5)	35(4)
C(9)	7258(5)	5393(10)	7050(5)	44(4)
C(10)	7334(5)	6391(11)	7501(5)	46(4)
C(11)	6600(7)	7185(9)	7521(5)	45(4)
C(12)	5789(6)	6981(9)	7089(5)	34(4)
C(13)	4375(10)	7348(14)	5686(7)	29(3)
C(14)	5151(10)	8126(14)	5557(7)	32(3)
C(15)	5350(11)	9291(15)	5878(8)	35(4)
C(16)	6020(11)	10069(16)	5728(8)	40(4)
C(17)	6485(10)	9685(15)	5277(7)	33(4)
C(18)	6286(9)	8525(14)	4947(7)	31(3)
C(19)	6808(10)	8087(16)	4456(8)	35(4)
C(20)	8389(7)	8108(10)	5482(4)	40(4)
C(25)	8835(8)	9205(11)	5331(4)	51(5)
C(24)	9250(8)	10024(9)	5826(6)	60(5)
C(23)	9219(8)	9745(11)	6473(5)	53(5)
C(22)	8773(9)	8648(12)	6624(4)	55(5)
C(21)	8358(8)	7830(10)	6129(5)	49(5)
C(26)	8501(6)	6958(11)	4233(4)	34(4)
C(31)	9202(7)	6074(11)	4377(5)	51(5)
C(30)	9809(7)	5938(11)	3959(6)	59(5)

C(29)	9714(7)	6684(12)	3397(5)	44(4)
C(28)	9012(8)	7567(11)	3253(4)	45(4)
C(27)	8406(7)	7704(10)	3670(5)	46(4)
F(1)	4643(9)	1628(12)	7783(6)	74(4)
F(2)	4187(8)	306(17)	6930(6)	93(5)
F(3)	5607(7)	164(12)	7472(6)	68(3)
F(4)	5173(9)	1887(12)	6837(6)	76(4)
B(1)	4905(13)	990(20)	7260(10)	45(5)
N(2)	7840(15)	10900(20)	4039(10)	76(5)
C(32)	9129(15)	12520(30)	4339(12)	80(6)
C(33)	8431(16)	11600(20)	4164(12)	68(5)

Table 3. Bond lengths [Å] and angles [°] for **Complex 5**.

Au(1)-Au(1)#1	2.9905(12)
Au(1)-Au(2)	3.2881(9)
Au(1)-P(1)#1	2.255(4)
Au(1)-N(1)	2.119(12)
Au(2)-Cl(1)	2.299(4)
Au(2)-P(2)	2.237(4)
P(1)-C(1)	1.820(8)
P(1)-C(7)	1.802(8)
P(1)-C(13)	1.857(16)
P(2)-C(19)	1.853(16)
P(2)-C(20)	1.811(9)
P(2)-C(26)	1.813(8)
N(1)-C(14)	1.367(13)
N(1)-C(18)	1.363(13)
C(1)-C(6)	1.3900
C(1)-C(2)	1.3900
C(6)-H(6)	0.9500
C(6)-C(5)	1.3900
C(5)-H(5)	0.9500
C(5)-C(4)	1.3900
C(4)-H(4)	0.9500
C(4)-C(3)	1.3900
C(3)-H(3)	0.9500

C(3)-C(2)	1.3900
C(2)-H(2)	0.9500
C(7)-C(8)	1.3900
C(7)-C(12)	1.3900
C(8)-H(8)	0.9500
C(8)-C(9)	1.3900
C(9)-H(9)	0.9500
C(9)-C(10)	1.3900
C(10)-H(10)	0.9500
C(10)-C(11)	1.3900
C(11)-H(11)	0.9500
C(11)-C(12)	1.3900
C(12)-H(12)	0.9500
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(13)-C(14)	1.49(2)
C(14)-C(15)	1.39(2)
C(15)-H(15)	0.9500
C(15)-C(16)	1.38(2)
C(16)-H(16)	0.9500
C(16)-C(17)	1.34(2)
C(17)-H(17)	0.9500
C(17)-C(18)	1.39(2)
C(18)-C(19)	1.48(2)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(25)	1.3900
C(20)-C(21)	1.3900
C(25)-H(25)	0.9500
C(25)-C(24)	1.3900
C(24)-H(24)	0.9500
C(24)-C(23)	1.3900
C(23)-H(23)	0.9500
C(23)-C(22)	1.3900
C(22)-H(22)	0.9500
C(22)-C(21)	1.3900
C(21)-H(21)	0.9500
C(26)-C(31)	1.3900
C(26)-C(27)	1.3900

C(31)-H(31)	0.9500
C(31)-C(30)	1.3900
C(30)-H(30)	0.9500
C(30)-C(29)	1.3900
C(29)-H(29)	0.9500
C(29)-C(28)	1.3900
C(28)-H(28)	0.9500
C(28)-C(27)	1.3900
C(27)-H(27)	0.9500
F(1)-B(1)	1.40(2)
F(2)-B(1)	1.37(2)
F(3)-B(1)	1.37(2)
F(4)-B(1)	1.39(3)
N(2)-C(33)	1.14(3)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(32)-C(33)	1.42(3)

Au(1)#1-Au(1)-Au(2)	95.71(3)
P(1)#1-Au(1)-Au(1)#1	81.48(10)
P(1)#1-Au(1)-Au(2)	88.22(10)
N(1)-Au(1)-Au(1)#1	111.0(3)
N(1)-Au(1)-Au(2)	89.8(3)
N(1)-Au(1)-P(1)#1	167.5(3)
Cl(1)-Au(2)-Au(1)	106.95(11)
P(2)-Au(2)-Au(1)	82.36(10)
P(2)-Au(2)-Cl(1)	170.43(15)
C(1)-P(1)-Au(1)#1	105.6(4)
C(1)-P(1)-C(13)	106.3(6)
C(7)-P(1)-Au(1)#1	116.7(3)
C(7)-P(1)-C(1)	105.3(5)
C(7)-P(1)-C(13)	105.5(6)
C(13)-P(1)-Au(1)#1	116.5(5)
C(19)-P(2)-Au(2)	117.7(5)
C(20)-P(2)-Au(2)	111.5(4)
C(20)-P(2)-C(19)	103.9(7)
C(20)-P(2)-C(26)	106.5(5)
C(26)-P(2)-Au(2)	110.2(4)

C(26)-P(2)-C(19)	106.3(6)
C(14)-N(1)-Au(1)	122.6(9)
C(18)-N(1)-Au(1)	117.4(9)
C(18)-N(1)-C(14)	120.0(13)
C(6)-C(1)-P(1)	123.0(6)
C(6)-C(1)-C(2)	120.0
C(2)-C(1)-P(1)	117.0(6)
C(1)-C(6)-H(6)	120.0
C(1)-C(6)-C(5)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-C(6)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(4)-H(4)	120.0
C(5)-C(4)-C(3)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-C(4)	120.0
C(2)-C(3)-H(3)	120.0
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-C(1)	120.0
C(3)-C(2)-H(2)	120.0
C(8)-C(7)-P(1)	120.7(5)
C(8)-C(7)-C(12)	120.0
C(12)-C(7)-P(1)	119.3(5)
C(7)-C(8)-H(8)	120.0
C(7)-C(8)-C(9)	120.0
C(9)-C(8)-H(8)	120.0
C(8)-C(9)-H(9)	120.0
C(8)-C(9)-C(10)	120.0
C(10)-C(9)-H(9)	120.0
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-C(9)	120.0
C(11)-C(10)-H(10)	120.0
C(10)-C(11)-H(11)	120.0
C(10)-C(11)-C(12)	120.0
C(12)-C(11)-H(11)	120.0
C(7)-C(12)-H(12)	120.0
C(11)-C(12)-C(7)	120.0

C(11)-C(12)-H(12)	120.0
P(1)-C(13)-H(13A)	108.3
P(1)-C(13)-H(13B)	108.3
H(13A)-C(13)-H(13B)	107.4
C(14)-C(13)-P(1)	115.8(10)
C(14)-C(13)-H(13A)	108.3
C(14)-C(13)-H(13B)	108.3
N(1)-C(14)-C(13)	120.9(13)
N(1)-C(14)-C(15)	119.7(14)
C(15)-C(14)-C(13)	119.3(13)
C(14)-C(15)-H(15)	120.0
C(16)-C(15)-C(14)	120.0(15)
C(16)-C(15)-H(15)	120.0
C(15)-C(16)-H(16)	120.1
C(17)-C(16)-C(15)	119.7(16)
C(17)-C(16)-H(16)	120.1
C(16)-C(17)-H(17)	119.6
C(16)-C(17)-C(18)	120.8(15)
C(18)-C(17)-H(17)	119.6
N(1)-C(18)-C(17)	119.8(13)
N(1)-C(18)-C(19)	119.2(13)
C(17)-C(18)-C(19)	121.0(13)
P(2)-C(19)-H(19A)	109.4
P(2)-C(19)-H(19B)	109.4
C(18)-C(19)-P(2)	111.4(11)
C(18)-C(19)-H(19A)	109.4
C(18)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
C(25)-C(20)-P(2)	120.1(6)
C(25)-C(20)-C(21)	120.0
C(21)-C(20)-P(2)	119.8(6)
C(20)-C(25)-H(25)	120.0
C(24)-C(25)-C(20)	120.0
C(24)-C(25)-H(25)	120.0
C(25)-C(24)-H(24)	120.0
C(25)-C(24)-C(23)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-C(24)	120.0

C(22)-C(23)-H(23)	120.0
C(23)-C(22)-H(22)	120.0
C(21)-C(22)-C(23)	120.0
C(21)-C(22)-H(22)	120.0
C(20)-C(21)-H(21)	120.0
C(22)-C(21)-C(20)	120.0
C(22)-C(21)-H(21)	120.0
C(31)-C(26)-P(2)	115.6(6)
C(31)-C(26)-C(27)	120.0
C(27)-C(26)-P(2)	124.4(6)
C(26)-C(31)-H(31)	120.0
C(26)-C(31)-C(30)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-C(31)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(29)-H(29)	120.0
C(30)-C(29)-C(28)	120.0
C(28)-C(29)-H(29)	120.0
C(29)-C(28)-H(28)	120.0
C(27)-C(28)-C(29)	120.0
C(27)-C(28)-H(28)	120.0
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-C(26)	120.0
C(28)-C(27)-H(27)	120.0
F(2)-B(1)-F(1)	108.8(16)
F(2)-B(1)-F(3)	109.0(18)
F(2)-B(1)-F(4)	109.0(17)
F(3)-B(1)-F(1)	111.3(16)
F(3)-B(1)-F(4)	108.6(15)
F(4)-B(1)-F(1)	110.1(17)
H(32A)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(33)-C(32)-H(32A)	109.5
C(33)-C(32)-H(32B)	109.5
C(33)-C(32)-H(32C)	109.5
N(2)-C(33)-C(32)	176(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Complex 5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	31(1)	25(1)	30(1)	-3(1)	8(1)	-1(1)
Au(2)	33(1)	28(1)	36(1)	2(1)	7(1)	0(1)
Cl(1)	45(2)	27(2)	45(2)	3(2)	3(2)	1(2)
P(1)	28(2)	31(2)	27(2)	-2(2)	7(2)	0(2)
P(2)	28(2)	35(2)	36(2)	3(2)	8(2)	-1(2)
N(1)	30(7)	25(7)	35(7)	-2(6)	10(6)	4(5)
C(1)	27(7)	33(8)	29(8)	-11(7)	4(6)	-2(7)
C(6)	45(10)	46(11)	46(10)	0(9)	6(8)	10(9)
C(5)	45(10)	61(13)	53(12)	-15(10)	8(9)	2(10)
C(4)	49(10)	48(11)	50(11)	-5(9)	24(9)	-21(9)
C(3)	63(12)	37(10)	51(11)	-8(9)	29(9)	-7(9)
C(2)	49(10)	45(10)	33(9)	-4(8)	15(8)	-5(8)
C(7)	31(8)	21(7)	37(9)	-1(7)	11(7)	-2(6)
C(8)	36(8)	33(9)	32(8)	-14(7)	-2(7)	-6(7)
C(9)	30(8)	51(11)	48(10)	-6(9)	1(7)	-4(8)
C(10)	43(10)	47(11)	44(10)	12(9)	0(8)	-5(9)
C(11)	52(11)	39(10)	45(10)	-9(8)	15(8)	-11(9)
C(12)	27(8)	36(9)	37(9)	-3(7)	1(7)	3(7)
C(13)	28(8)	28(8)	30(8)	-8(7)	7(6)	-2(6)
C(14)	38(9)	21(8)	39(9)	1(7)	9(7)	3(7)
C(15)	46(9)	26(8)	33(9)	9(7)	9(7)	10(7)
C(16)	46(9)	26(8)	45(10)	-4(8)	5(8)	-4(8)
C(17)	33(8)	29(8)	38(9)	-4(7)	5(7)	-5(7)
C(18)	33(8)	20(8)	39(9)	3(7)	3(7)	6(7)
C(19)	38(9)	32(9)	37(9)	8(7)	9(7)	0(7)
C(20)	34(9)	49(11)	41(9)	-1(8)	21(7)	-5(8)
C(25)	60(12)	41(11)	52(11)	-6(9)	9(9)	-14(10)
C(24)	71(13)	43(11)	67(14)	-4(11)	12(11)	-9(11)
C(23)	55(11)	39(11)	58(12)	-23(9)	-6(9)	2(9)
C(22)	67(13)	56(13)	41(11)	-7(9)	7(9)	0(11)

C(21)	56(11)	56(12)	36(10)	3(9)	10(8)	-7(10)
C(26)	37(9)	42(9)	24(8)	-12(7)	14(7)	-8(8)
C(31)	34(9)	73(14)	45(11)	20(10)	5(8)	7(9)
C(30)	55(12)	69(14)	59(13)	3(11)	23(10)	19(11)
C(29)	48(10)	40(10)	47(11)	1(9)	18(8)	-3(9)
C(28)	55(11)	42(10)	42(10)	9(8)	19(8)	-4(9)
C(27)	45(10)	47(11)	47(11)	6(9)	14(8)	2(9)
F(1)	95(9)	59(8)	77(8)	-17(7)	43(7)	5(7)
F(2)	54(7)	165(16)	64(8)	-32(9)	26(6)	-25(9)
F(3)	55(7)	62(8)	91(9)	19(7)	23(6)	15(6)
F(4)	99(10)	55(7)	92(9)	9(7)	62(8)	16(7)
B(1)	38(11)	54(13)	43(11)	-14(10)	6(9)	0(10)
N(2)	98(13)	61(11)	72(11)	2(10)	18(11)	-3(8)
C(32)	54(11)	88(14)	90(14)	21(13)	-3(11)	10(8)
C(33)	70(12)	65(12)	72(11)	14(10)	22(10)	10(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **Complex 5**.

	x	y	z	U(eq)
H(6)	2893	6783	6197	55
H(5)	1859	6268	6859	64
H(4)	2184	4618	7633	57
H(3)	3542	3483	7745	57
H(2)	4576	3997	7083	49
H(8)	6396	4506	6309	42
H(9)	7761	4850	7037	53
H(10)	7888	6531	7797	55
H(11)	6651	7867	7830	53
H(12)	5287	7523	7102	41
H(13A)	3951	7213	5267	35
H(13B)	4055	7857	5972	35
H(15)	5024	9553	6202	42
H(16)	6151	10874	5942	48
H(17)	6956	10213	5181	40
H(19A)	7021	8847	4242	42
H(19B)	6412	7575	4116	42
H(25)	8856	9395	4889	61
H(24)	9555	10773	5722	72
H(23)	9503	10305	6811	64
H(22)	8752	8458	7066	66
H(21)	8054	7080	6233	59
H(31)	9267	5565	4761	61
H(30)	10288	5334	4058	71
H(29)	10129	6590	3112	53
H(28)	8947	8077	2868	54
H(27)	7926	8307	3571	55
H(32A)	9559	12443	4044	119
H(32B)	9441	12367	4789	119
H(32C)	8870	13391	4303	119

Table 6. Torsion angles [°] for **Complex 5**.

Au(1)#1-P(1)-C(1)-C(6)	-107.8(6)
Au(1)#1-P(1)-C(1)-C(2)	70.9(6)
Au(1)#1-P(1)-C(7)-C(8)	3.9(7)
Au(1)#1-P(1)-C(7)-C(12)	-177.1(5)
Au(1)#1-P(1)-C(13)-C(14)	-94.5(11)
Au(1)-N(1)-C(14)-C(13)	-7(2)
Au(1)-N(1)-C(14)-C(15)	177.3(11)
Au(1)-N(1)-C(18)-C(17)	-176.7(11)
Au(1)-N(1)-C(18)-C(19)	0.4(18)
Au(2)-P(2)-C(19)-C(18)	69.3(12)
Au(2)-P(2)-C(20)-C(25)	162.4(6)
Au(2)-P(2)-C(20)-C(21)	-21.4(8)
Au(2)-P(2)-C(26)-C(31)	-41.3(7)
Au(2)-P(2)-C(26)-C(27)	141.5(6)
P(1)-C(1)-C(6)-C(5)	178.7(8)
P(1)-C(1)-C(2)-C(3)	-178.7(8)
P(1)-C(7)-C(8)-C(9)	178.9(8)
P(1)-C(7)-C(12)-C(11)	-178.9(8)
P(1)-C(13)-C(14)-N(1)	68.4(17)
P(1)-C(13)-C(14)-C(15)	-116.1(14)
P(2)-C(20)-C(25)-C(24)	176.2(9)
P(2)-C(20)-C(21)-C(22)	-176.2(9)
P(2)-C(26)-C(31)-C(30)	-177.3(8)
P(2)-C(26)-C(27)-C(28)	177.0(9)
N(1)-C(14)-C(15)-C(16)	1(2)
N(1)-C(18)-C(19)-P(2)	-86.9(15)
C(1)-P(1)-C(7)-C(8)	120.6(6)
C(1)-P(1)-C(7)-C(12)	-60.5(7)
C(1)-P(1)-C(13)-C(14)	148.3(10)
C(1)-C(6)-C(5)-C(4)	0.0
C(6)-C(1)-C(2)-C(3)	0.0
C(6)-C(5)-C(4)-C(3)	0.0
C(5)-C(4)-C(3)-C(2)	0.0
C(4)-C(3)-C(2)-C(1)	0.0
C(2)-C(1)-C(6)-C(5)	0.0
C(7)-P(1)-C(1)-C(6)	128.2(7)
C(7)-P(1)-C(1)-C(2)	-53.1(7)

C(7)-P(1)-C(13)-C(14)	36.7(12)
C(7)-C(8)-C(9)-C(10)	0.0
C(8)-C(7)-C(12)-C(11)	0.0
C(8)-C(9)-C(10)-C(11)	0.0
C(9)-C(10)-C(11)-C(12)	0.0
C(10)-C(11)-C(12)-C(7)	0.0
C(12)-C(7)-C(8)-C(9)	0.0
C(13)-P(1)-C(1)-C(6)	16.5(8)
C(13)-P(1)-C(1)-C(2)	-164.8(7)
C(13)-P(1)-C(7)-C(8)	-127.2(7)
C(13)-P(1)-C(7)-C(12)	51.7(8)
C(13)-C(14)-C(15)-C(16)	-175.0(15)
C(14)-N(1)-C(18)-C(17)	2(2)
C(14)-N(1)-C(18)-C(19)	178.7(13)
C(14)-C(15)-C(16)-C(17)	-1(2)
C(15)-C(16)-C(17)-C(18)	2(2)
C(16)-C(17)-C(18)-N(1)	-2(2)
C(16)-C(17)-C(18)-C(19)	-179.0(15)
C(17)-C(18)-C(19)-P(2)	90.2(16)
C(18)-N(1)-C(14)-C(13)	174.6(13)
C(18)-N(1)-C(14)-C(15)	-1(2)
C(19)-P(2)-C(20)-C(25)	-69.9(8)
C(19)-P(2)-C(20)-C(21)	106.3(8)
C(19)-P(2)-C(26)-C(31)	-169.9(8)
C(19)-P(2)-C(26)-C(27)	13.0(10)
C(20)-P(2)-C(19)-C(18)	-54.6(12)
C(20)-P(2)-C(26)-C(31)	79.8(7)
C(20)-P(2)-C(26)-C(27)	-97.3(8)
C(20)-C(25)-C(24)-C(23)	0.0
C(25)-C(20)-C(21)-C(22)	0.0
C(25)-C(24)-C(23)-C(22)	0.0
C(24)-C(23)-C(22)-C(21)	0.0
C(23)-C(22)-C(21)-C(20)	0.0
C(21)-C(20)-C(25)-C(24)	0.0
C(26)-P(2)-C(19)-C(18)	-166.7(10)
C(26)-P(2)-C(20)-C(25)	42.1(8)
C(26)-P(2)-C(20)-C(21)	-141.7(7)
C(26)-C(31)-C(30)-C(29)	0.0
C(31)-C(26)-C(27)-C(28)	0.0

C(31)-C(30)-C(29)-C(28)	0.0
C(30)-C(29)-C(28)-C(27)	0.0
C(29)-C(28)-C(27)-C(26)	0.0
C(27)-C(26)-C(31)-C(30)	0.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 7. Hydrogen bonds for **Complex 5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9)...F(3)#2	0.95	2.50	3.197(14)	129.9
C(29)-H(29)...F(3)#3	0.95	2.45	3.199(15)	136.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+3/2,y+1/2,-z+3/2 #3 x+1/2,-y+1/2,z-1/2