

Electronic supplementary information for the paper

**First structurally confirmed example of the formation of a gold(III) carbon bond via
transmetallation with a boroxine.**

Gregory A. Price,^a Kevin R. Flower,^{*a} Robin G. Pritchard,^a

Alan K. Brisdon,^a and Peter Quayle^a

^aSchool of Chemistry
The University of Manchester
Oxford Road
Manchester
UK
M13 9PL

Experimental Section

General Considerations: Diethyl ether was dried by refluxing over sodium-potassium alloy and distilled prior to use. Tetrahydrofuran was dried by refluxing over potassium and distilled prior to use. Chemicals and compounds whose syntheses are not mentioned were obtained from commercial sources and used as received. ¹H-NMR spectra were recorded on either a Bruker Avance III (400.1 MHz) or a Bruker DPX300 (300 MHz). ¹³C {¹H}-NMR were recorded on either a Bruker Avance III (100.6 MHz) or a Bruker DPX300 (75.4 MHz), and ¹¹B {¹H} -NMR were recorded on a Bruker Avance III (128.4 MHz). ¹H and {¹H}-¹³C NMR spectra were referenced to solvent signals and ¹¹B {¹H} to boric acid. Elemental analyses were performed by the Microanalytical Service, The University of Manchester, Manchester, UK. All air and moisture sensitive procedures were carried out under an atmosphere of argon using standard Schlenk techniques.

Syntheses

Preparation of 2-(Me₂NCH₂)C₆H₄Li

Prepared following the procedure of Manzer.¹ To N,N-dimethylbenzylamine (2.4 mL, 16 mmol) in Et₂O (15 mL) under argon was added *n*-butyllithium (10 mL, 16 mmol, 1.6 M in hexanes) and the mixture stirred for 24 h. The white precipitate was filtered under argon, washed with Et₂O (3 x 10 mL) and dried *in vacuo*. It was then transferred to a glovebox for storage.

Typical yield 1.95g, 89%

Preparation of (2-(Me₂NCH₂)C₆H₄BO)₃ (**1**)²

To a stirred solution of 2-(Me₂NCH₂)C₆H₄Li (5g, 35.5 mmol) in THF (20 mL) at -78°C was added B(OMe)₃ (6.3 mL, 49.2 mmol) and the solution stirred for 1 h before warming to room temperature overnight. The solution was acidified with 1M HCl and brine was added. The phases were separated, the aqueous layer washed with Et₂O and all organic phases combined and washed with saturated Na₂CO₃ solution and brine. The organic layer was dried over MgSO₄ and the solvent evaporated to give (2-(Me₂NCH₂)C₆H₄BO)₃ (**1**) which was recrystallised from dichloromethane/hexane.

Yield 2.9 g, 50%

Elemental Analysis: Calculated for C₂₇H₃₆N₃B₃O₃: C, 67.0; H, 7.5; N, 8.7; B, 6.8; Found: C, 66.4; H, 7.6; N, 8.6; B, 6.8; ¹H NMR (CDCl₃, δ ppm): 7.65 (dd, *J*=5.0, 3.5 Hz, 3H, Ph-H), 7.13 - 7.36 (m, 9H, Ph-H), 3.88 (s, 6H, CH₂), 2.46 (s, 18H, NMe₂). ¹³C NMR {¹H}(CDCl₃):

(C-B not observed) 141.4, 131.6, 127.2, 126.6, 124.9 (Ph-C), 64.0 (CH₂), 45.1 (CH₃). ¹¹B{¹H}
NMR (CDCl₃, δ ppm): = 16.6 (s).

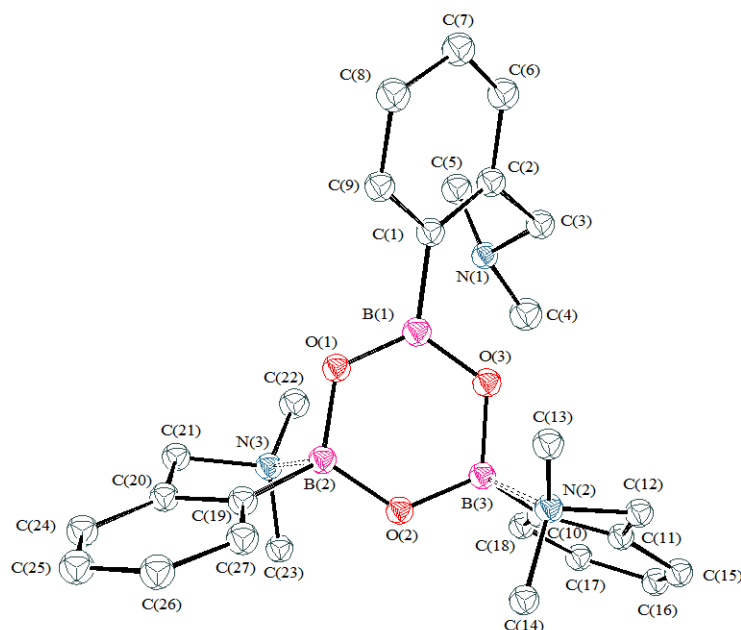


Figure S1: An ORTEP³ representation of the molecular structure of (2-(Me₂NCH₂)C₆H₄BO)₃ **1**, showing the atomic numbering scheme and thermal ellipsoids are shown at 30% probability level.

Preparation of 2-[(Dimethylamino)methyl]phenylgold(III)dichloride (**5**)⁴

To a solution of Na[AuCl₄]·2H₂O (0.2 g, 0.50 mmol) in H₂O (25 mL) was added (2-(Me₂NCH₂)C₆H₄BO)₃ **1** (0.08 g, 0.17 mmol) in MeCN (5 mL). The yellow mixture was refluxed for 48 h. The acetonitrile was removed under reduced pressure, the mixture filtered and the solid extracted into CH₂Cl₂ (10 mL) and hexane (15 mL) added. The CH₂Cl₂ was removed slowly under reduced pressure to induce crystallisation of [Au(III)(damp-C,N)Cl₂] (**2**) which was collected by filtration.

Yield 0.1 g, 57%

Elemental Analysis: Calculated for $C_9H_{12}NAuCl_2$: C, 26.9; H, 3.0; N, 3.5

Found: C, 26.9; H, 2.7; N, 3.2. 1H NMR ($CDCl_3$): 7.68 (d, $J=7.6$ Hz, 1 H, Ph-H), 7.15 - 7.31 (m, 2 H, Ph-H), 7.04 - 7.14 (m, 1 H, Ph-H), 4.34 (s, 2 H, CH_2), 3.26 (s, 6 H, NMe_2). $^{13}C\{^1H\}$ NMR ($CDCl_3$): 148.0 (Ph-C), 143.6 (Ph-C), 131.3 (Ph-C), 129.1 (Ph-C), 128.1 (Ph-C), 123.2 (Ph-C), 75.9 (CH_2), 53.8 (NMe_2).

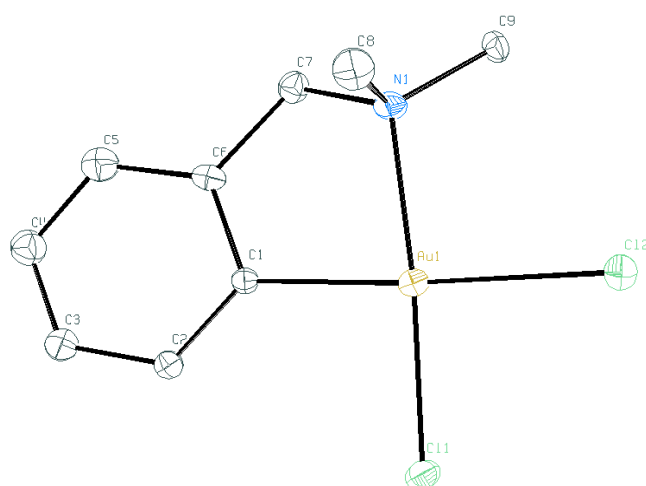


Figure S2: An ORTEP³ representation of the molecular structure of 2-[(Dimethylamino)methyl]phenylgold(III) **2**, showing the atomic numbering scheme and thermal ellipsoids are shown at 30% probability level.

Preparation of 4-(Me_2NCH_2) $C_6H_4CF_3$ ⁵

To a solution of 4-($BrCH_2$) $C_6H_4CF_3$ (20 g, 84 mmol) in dichloromethane (150 mL) was added an aqueous solution of dimethylamine hydrochloride (52 g, 0.6 mol) and potassium hydroxide (70.4 g, 1.3 mol) at room temperature. After stirring for 4.5 h the organic phase was separated, washed with brine (3 x 25 mL) and dried over $MgSO_4$. The solvent was removed *in vacuo* to give 4-(Me_2NCH_2) $C_6H_4CF_3$.

Yield 15.2 g, 89%

Elemental Analysis: Calculated for $C_{10}H_{12}F_3N$: C, 59.1; H, 6.0; N, 6.9

Found: C, 59.2; H, 5.6; N, 6.9.

1H NMR ($CDCl_3$): δ = 7.49 (d, $J=8.1$ Hz, 2 H, Ph-H), 7.35 (d, $J=8.1$ Hz, 2 H, Ph-H), 3.38 (s, 2 H, CH_2), 2.16 ppm (s, 6 H, NMe_2). 143.3 (q, $J_{CF}=1.35$ Hz, Ph-C); 129.3 (q, $^2J_{CF}=32.24$ Hz, Ph-C); 129.1 (s, Ph-C); 125.1 (q, $J_{CF}=3.84$ Hz, Ph-C); 124.3 (q, $^1J_{CF}=271.83$ Hz, CF_3); 63.8 (s, CH_2); 45.4 (s, NMe_2).

Preparation of 2-(Me_2NCH_2)-5- CF_3 - C_6H_4Li

To 4-(Me_2NCH_2) $C_6H_4CF_3$ (12.4 g, 61.3 mmol) in hexane (30 mL) under argon was added *n*-butyllithium (42.1 mL, 67.4 mmol, 1.6 M in hexanes) and the mixture was stirred for 48 hours. The white precipitate was filtered under argon, washed with hexane (3 x 15 mL) and dried *in vacuo*. It was then transferred to a glovebox for storage.

Yield 9 g, 70%

Preparation of (2-(Me_2NCH_2)-5- $CF_3C_6H_4BO$)₃ (2)

To a stirred solution of 2-(Me_2NCH_2)-5- $CF_3C_6H_4Li$ (3.2 g, 15.3 mmol) in THF (20 mL) at -78 °C was added $B(OMe)_3$ (2.6 mL, 23 mmol) and the solution stirred for 1 h before warming to room temperature overnight. The solution was acidified with 1M HCl and brine was added. The phases were separated and the aqueous layer neutralised with 1M NaOH. The aqueous layer was extracted with dichloromethane the phases separated, and the combined organic fractions dried over $MgSO_4$. The solvent was removed *in vacuo* to give (2-(Me_2NCH_2)-5- $CF_3C_6H_4BO$)₃ which was recrystallised from dichloromethane/hexane.

Yield 2.3 g, 66%

Elemental Analysis: Calculated for $C_{30}H_{33}B_3F_9N_3O_3$: C, 52.4; H, 4.8; N, 6.1

Found: C, 52.6; H, 4.7; N, 6.1. 1H NMR ($CDCl_3$): δ = 7.84 (s, 3 H, Ph-H), 7.50 (d, J =7.7 Hz, 3 H, Ph-H), 7.27 (d, J =8.3 Hz, 3 H, Ph-H), 3.89 (s, 6 H, CH_2), 2.45 (s, 18 H, NMe_2). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ = (C-B not observed), 145.08 (s, Ph-C); 128.9 (q, $^2J_{CF}$ =31.1 Hz, Ph-C); 127.9 (q, J_{CF} =3.5 Hz, Ph-C); 125 (s, Ph-C); 124.9 (q, $^1J_{CF}$ = 272.1 Hz, CF_3); 124.3 (q, $^3J_{CF}$ =3.7 Hz, Ph-C). $^{11}B\{^1H\}$ NMR ($CDCl_3$, δ ppm): 14.32 (s).

Preparation of 2- Me_2NCH_2 -5- CF_3 - $C_6H_4AuCl_2$ (6)

To a solution of $Na[AuCl_4] \cdot 2H_2O$ (0.2 g, 0.5 mmol) in H_2O (25 mL) was added (2- (Me_2NCH_2) -5- CF_3 - C_6H_4BO)₃ (0.1 g, 0.2 mmol) in MeCN (5 mL). The yellow mixture was refluxed for 48 h. The acetonitrile was removed under reduced pressure, the mixture filtered and the solid extracted into CH_2Cl_2 (10 mL) and hexane (15 mL) added. The CH_2Cl_2 was removed slowly under reduced pressure to induce crystallisation of 2- Me_2NCH_2 -5- $CF_3C_6H_4AuCl_2$ which was collected by filtration.

Yield 0.1 g, 63%

Elemental Analysis: Calculated for $C_{10}H_{11}AuCl_2F_3N$: C, 25.5; H, 2.4; N, 3.0

Found: C, 25.5; H, 2.0; N, 2.9.

1H NMR (d^6 -DMSO): δ = 7.98 (s, 1 H), 7.47 (d, J =7.9 Hz, 1 H), 7.10 - 7.30 (m, 1 H), 4.41 (s, 2 H), 3.28 (s, 6 H). $^{13}C\{^1H\}$ NMR (d^6 -DMSO): δ = 151.1 (s, Ph-C); 146.51 (s, Ph-C); 126.9 (q, $^2J_{CF}$ = 31.6 Hz, Ph-C); 125.8 (q, J_{CF} = 4.0 Hz, Ph-C); 125.3 (q, J_{CF} = 3.9 Hz, Ph-C); 124.60 (s, Ph-C); 123.7 (q, $^1J_{CF}$ = 272.7 Hz, CF_3); 74.2 (s, CH_2); 53.3 (s, NMe_2).

Preparation of 1- Me_2NCH_2 -4- CH_3 - C_6H_4

To a solution of 1-BrCH₂-4-CH₃-C₆H₄ (20 g, 0.1 mol) in dichloromethane (150 mL) was added an aqueous solution of dimethylamine hydrochloride (61.7 g, 0.8 mol) in the presence of KOH (84.9 g, 1.5 mol) at room temperature. After stirring for 4.5 h the organic phase was separated and dried over MgSO₄. Removal of the solvent afforded 1-Me₂NCH₂-4-CH₃-C₆H₄. Yield 10 g, 61%

Elemental Analysis: Calculated for C₁₀H₁₅N: C, 80.5; H, 10.1; N, 9.4

Found: C, 79.9; H, 10.0; N, 9.1. ¹H NMR (CDCl₃): δ = 6.91 - 7.17 (m, 4 H, Ph-H), 3.29 (s, 2 H, CH₂), 2.25 (s, 3 H, CH₃), 2.14 ppm (s, 6 H, NMe₂). ¹³C{¹H} NMR (CDCl₃): δ = 136.6, 135.9, 129.1, 128.9 (Ph-C), 64.2 (CH₂), 45.3 (NMe₂), 21.1 (CH₃) ppm.

Preparation of 2-(Me₂NCH₂)-5-CH₃-C₆H₃Li⁶

To a solution of 1-Me₂NCH₂-4-CH₃-C₆H₄ (7.2 g, 48 mmol) in Et₂O (125 mL) was added *n*-Butyllithium (36.2 mL, 58 mmol, 1.6 M in hexanes) and the mixture was stirred for 3 days. The solution was concentrated to 30 mL and cooled to -20 °C for 24 h. The white precipitate that had formed was filtered under argon, washed with cold hexane (2 x 10 mL) and transferred to a glovebox for storage.

Yield 4.5 g, 61%

Preparation of (2-(Me₂NCH₂)-5-CH₃-C₆H₄BO)₃ (3)

To a stirred solution of 2-(Me₂NCH₂)-5-CH₃-C₆H₄Li (2.8 g, 18 mmol) in THF (20 mL) at -78 °C was added B(OMe)₃ (3.0 mL, 27.1 mmol) and the solution stirred for 1 h before warming to room temperature overnight. The solution was acidified with 1M HCl and brine was added.

The phases were separated and the aqueous layer neutralised with 1M NaOH. The aqueous layer was extracted with dichloromethane the phases separated, and the combined organic fractions dried over MgSO₄. The solvent was removed *in vacuo* to give (2-(Me₂NCH₂)-5-CH₃-C₆H₄BO)₃ which was recrystallised from dichloromethane/hexane.

Yield 2.2 g, 68%

Elemental Analysis: Calculated for C₃₀H₄₂B₃N₃O₃: C, 68.5; H, 8.1; N, 8.0

Found: C, 68.3; H, 8.3; N, 7.9. ¹H NMR (CDCl₃): δ = 7.36 (s, 3 H, Ph-H), 6.96 (s, 6 H, Ph-H), 3.75 (s, 6 H, CH₂), 2.35 (s, 18 H, NMe₂), 2.26 ppm (s, 9 H, CH₃). ¹³C{¹H} NMR: δ = 138.5, 135.7, 132.4, 127.9, 124.8 (Ph-C), 63.8 (CH₂), 45.1 (NMe₂), 21.5 (CH₃) ppm. ¹¹B{¹H} NMR (CDCl₃, δ ppm): 15.12 (s).

Preparation of 2-Me₂NCH₂-5-CH₃-C₆H₄AuCl₂ (7)

To Na[AuCl₄]. 2H₂O (0.2 g, 0.50 mmol) in H₂O (25 mL) was added (2-(Me₂NCH₂)-5-CH₃C₆H₄BO)₃ (0.1 g, 0.2 mmol) in acetonitrile (5 mL). The yellow mixture was refluxed for 48 h. The acetonitrile was removed under reduced pressure, the mixture filtered and the solid extracted into CH₂Cl₂ (10 mL) and hexane (15 mL) added. The CH₂Cl₂ was removed slowly under reduced pressure to induce crystallisation of 2-Me₂NCH₂-5-CH₃-C₆H₄AuCl₂ which was collected by filtration.

Yield 0.12 g, 58%

Elemental Analysis: Calculated for C₁₀H₁₄AuCl₂N: C, 28.9; H, 3.4; N, 3.4

Found: C, 29.9; H, 3.1; N, 3.4. ¹H NMR (CDCl₃): δ = 7.49 (s, 1 H, Ph-H), 6.85 - 7.08 (m, 2 H, Ph-H), 4.28 (s, 2 H, CH₂), 3.24 (s, 6 H, NMe₂), 2.29 (s, 3 H, CH₃). ¹³C{¹H} NMR: δ = 148.1, 140.4, 138.4, 131.7, 129.6, 122.8 (Ph-C), 75.7 (CH₂), 53.7 (NMe₂), 21.5(CH₃).

Preparation of 1-Me₂NCH₂-4-OMe-C₆H₄

To a solution of 4-(ClCH₂)C₆H₄OMe (20 g, 0.13 mol) in dichloromethane (150 mL) was added an aqueous solution of dimethylamine hydrochloride (78.1 g, 1 mol) in the presence of potassium hydroxide (107.3 g, 1.9 mol) at room temperature. After stirring for 4.5 h the organic phase was separated, washed with brine and dried over MgSO₄. The solvent was removed to afford 1-Me₂NCH₂-4-OMe-C₆H₄.

Yield 17.7 g, 85%

Elemental Analysis: Calculated for C₁₀H₁₅NO: C, 72.7; H, 9.2; N, 8.5

Found: C, 72.4; H, 9.5; N, 8.4. ¹H NMR (CDCl₃): δ = 7.21 (d, *J* = 8.7 Hz, 2 H, Ph-H), 6.85 (d, *J* = 8.7 Hz, 2 H, Ph-H), 3.76 (s, 3 H, OCH₃), 3.34 (s, 2 H, CH₂), 2.21 ppm (s, 6 H, NMe₂).
¹³C{¹H} NMR: δ = 158.7, 131.0, 130.2, 113.6 (Ph-C), 63.7 (CH₂), 55.1 (OCH₃), 45.2 (NMe₂) ppm.

Preparation of (2-(Me₂NCH₂)-5-OMe-C₆H₄BO)₃ (4)

To 1-Me₂NCH₂-4-OMe-C₆H₄ (3.6 g, 21.6 mmol) in Et₂O (25 mL) was added *n*-Butyllithium (14.8 mL, 23.7 mmol, 1.6M in hexanes) and the mixture stirred for 18 h at room temperature. The solution was added to a vigorously stirred solution of B(OMe)₃ (3.6 mL, 32.3 mmol) in Et₂O (20 mL) at -78°C and allowed to warm to room temperature overnight. The solution was acidified with 1M HCl and brine was added. The phases were separated and the aqueous layer neutralised with 1M NaOH. The aqueous layer was extracted with Et₂O the phases separated, and the combined organic fractions dried over MgSO₄. The solvent was removed *in vacuo* to give (2-(Me₂NCH₂)-5-OMe-C₆H₄BO)₃ which was recrystallised from dichloromethane/hexane.

Yield 1.9 g, 45%

Elemental Analysis: Calculated for $C_{30}H_{42}B_3N_3O_6$: C, 62.8; H, 7.4; N, 7.3

Found: C, 62.3; H, 7.4; N, 7.2. 1H NMR ($CDCl_3$): δ = 7.18 (d, J =2.6 Hz, 3 H, Ph-H), 7.08 (d, J =8.1 Hz, 3 H, Ph-H), 6.77 (dd, J =8.1, 2.6 Hz, 3 H, Ph-H), 3.81 (s, 15 H, CH_2 + OCH_3), 2.44 ppm (s, 18 H, NMe_2). $^{13}C\{^1H\}$ NMR: δ = 158.5, 133.6, 125.9, 117.1, 112.3 (Ph-C), 63.5 (CH_2), 55.2 (OCH_3), 45.0 (NMe_2) ppm. $^{11}B\{^1H\}$ NMR ($CDCl_3$, δ ppm): 16.84 (s).

Preparation of 2-Me₂NCH₂-5-OMe-C₆H₄AuCl₂ (8)

To $Na[AuCl_4] \cdot 2H_2O$ (0.2 g, 0.5 mmol) in H_2O (25 mL) was added (2-(Me₂NCH₂)-5-OMe-C₆H₄BO)₃ (0.1 g, 0.2 mmol) in MeCN (5 mL) and the mixture refluxed for 48 h. The acetonitrile was removed under reduced pressure, the mixture filtered and the solid extracted into CH_2Cl_2 (10 mL) and hexane added (15 mL). The CH_2Cl_2 was removed slowly under reduced pressure to induce crystallisation of 2-Me₂NCH₂-5-OMe-C₆H₄AuCl₂ which was collected by filtration.

Yield 0.08g, 35%

Elemental Analysis: Calculated for $C_{10}H_{14}AuCl_2NO$: C, 27.8; H, 3.3; N, 3.2

Found: C, 27.1; H, 3.0; N, 3.1. 1H NMR ($CDCl_3$): δ = 7.26 (d, J =2.4 Hz, 1 H, Ph-H), 6.99 (d, J =8.3 Hz, 1 H, Ph-H), 6.74 (dd, J =8.3, 2.4 Hz, 1 H, Ph-H), 4.28 (s, 2 H, CH_2), 3.74 (s, 3 H, OCH_3), 3.23 (s, 6 H, NMe_2). $^{13}C\{^1H\}$ NMR: δ = 157.9, 148.5, 135.5, 123.7, 115.7, 115.4 (Ph-C), 75.5 (CH_2), 55.6 (OCH_3), 53.7 (NMe_2).

X-Ray Crystallography

A suitable single crystal was coated in inert perfluoropolyether oil and mounted on a single glass wool strand of *ca.* 3 mm in length glued to a glass fibre.

The X-Ray crystallography measurements were recorded on a Bruker-Nonius Kappa CCD machine using MoK α radiation (λ = 0.71073 Å) at 100 K.

Data were corrected for Lorentz, polarisation and absorption using the multi-scan method.

The data for **1** and **5** showed the unit cells were equivalent to those previously reported see Table S1, and a preliminary solution (isotropic) was carried out to confirm connectivities, see figures S1 and S2; for previously unsolved **7** see Table S2 for crystal data and details of the structure determination and Tables S3 and S4 for Bond lengths (Å) and angles (°).

Table S1: Unit Cell dimensions for compounds **1** and **5**.

	1	Lit²	5	Lit⁴
α (°)	-	-	-	-
β (°)	-	-	100.2530(10)	100.22(3)
γ (°)	-	-	-	-
a (Å)	8.9650(6)	8.9765(3)	7.7340(3)	7.896(3)
b (Å)	14.709(1)	14.6975(4)	9.4210(3)	9.487(3)
c (Å)	19.517 (2)	19.6627(6)	15.0630(7)	15.107(6)

Table S2 - Crystal Data and Details of the Structure Determination
for: **7** P 21/c R = 0.05

Crystal Data				
Formula	C10	H14	Au1	Cl2 N1
Formula Weight				416.09
Crystal System				Monoclinic
Space group	P21/c			(No. 14)
a, b, c [Angstrom]	8.7402 (3)	11.1657 (5)		16.9401 (5)
alpha, beta, gamma [deg]	90	135.074 (2)		90
V [Ang**3]				1167.47 (8)
Z				4
D(calc) [g/cm**3]				2.367
Mu(MoKa) [/mm]				13.019
F(000)				776
Crystal Size [mm]	0.05 x	0.12 x		0.16
Data Collection				
Temperature (K)				100
Radiation [Angstrom]	MoKa			0.71073
Theta Min-Max [Deg]				3.0, 27.5
Dataset	-11: 11 ; -14: 13 ; -22: 21			
Tot., Uniq. Data, R(int)	8932,	2663,		0.051
Observed data [I > 0.0 sigma(I)]				2372
Refinement				
Nref, Npar		2663,		129
R, wR2, S	0.0469,	0.1202,		1.10
w = 1/[s^2^(Fo^2^)+(0.0362P)^2^+26.3388P] where P=(Fo^2^+2Fc^2^)/				
Max. and Av. Shift/Error				0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]				-2.28, 8.18

Table S3 - Bond Distances (Angstrom)

Au1-Cl1	2.385 (3)	C3-H3	0.9500
Au1-Cl2	2.287 (3)	C4-H4	0.9500
Au1-N1	2.091 (10)	C6-H6	0.9500
Au1-C1	2.028 (10)	C7-H7A	0.9900
N1-C7	1.484 (19)	C7-H7B	0.9900
N1-C8	1.490 (19)	C8-H8A	0.9800
N1-C9	1.486 (15)	C8-H8B	0.9800
C1-C2	1.393 (19)	C8-H8C	0.9800
C1-C6	1.394 (14)	C9-H9A	0.9800
C2-C3	1.385 (16)	C9-H9B	0.9800
C2-C7	1.502 (14)	C9-H9C	0.9800
C3-C4	1.375 (15)	C10-H10A	0.9800
C4-C5	1.41 (2)	C10-H10B	0.9800
C5-C6	1.372 (17)	C10-H10C	0.9800
C5-C10	1.541 (15)		

Table S4 - Bond Angles (°)

Cl1-Au1-Cl2	91.99 (9)	C3-C4-H4	120.00
Cl1-Au1-N1	94.1 (3)	C5-C4-H4	120.00
Cl1-Au1-C1	175.6 (3)	C1-C6-H6	120.00
Cl2-Au1-N1	173.8 (3)	C5-C6-H6	120.00
Cl2-Au1-C1	92.4 (3)	N1-C7-H7A	110.00
N1-Au1-C1	81.5 (4)	N1-C7-H7B	110.00
Au1-N1-C7	106.8 (6)	C2-C7-H7A	110.00
Au1-N1-C8	107.1 (9)	C2-C7-H7B	110.00
Au1-N1-C9	114.1 (7)	H7A-C7-H7B	108.00
C7-N1-C8	111.5 (9)	N1-C8-H8A	109.00
C7-N1-C9	108.8 (12)	N1-C8-H8B	109.00
C8-N1-C9	108.6 (9)	N1-C8-H8C	109.00

Au1-C1-C2	112.6 (6)	H8A-C8-H8B	110.00
Au1-C1-C6	126.5 (10)	H8A-C8-H8C	110.00
C2-C1-C6	120.7 (10)	H8B-C8-H8C	110.00
C1-C2-C3	118.5 (9)	N1-C9-H9A	109.00
C1-C2-C7	116.5 (9)	N1-C9-H9B	110.00
C3-C2-C7	125.0 (12)	N1-C9-H9C	109.00
C2-C3-C4	121.4 (13)	H9A-C9-H9B	109.00
C3-C4-C5	119.7 (11)	H9A-C9-H9C	109.00
C4-C5-C6	119.8 (10)	H9B-C9-H9C	109.00
C4-C5-C10	119.9 (11)	C5-C10-H10A	109.00
C6-C5-C10	120.4 (12)	C5-C10-H10B	109.00
C1-C6-C5	119.9 (12)	C5-C10-H10C	109.00
N1-C7-C2	108.7 (11)	H10A-C10-H10B	109.00
C2-C3-H3	119.00	H10A-C10-H10C	110.00
C4-C3-H3	119.00	H10B-C10-H10C	109.00

References

1. L. E. Manzer, *J. Am. Chem. Soc.*, 1978, **100**, 8068-8073.
2. J. C. Norrild and I. Sotofte, *J. Chem. Soc.-Perkin Trans. 2*, 2002, 303-311.
3. L. J. Farrugia, *ORTEP 3 for windows*, University of Glasgow
4. J. Mack, K. Ortner and U. Abram, *Z. Anorg. Allg. Chem.*, 1997, **623**, 873-879.
5. E. Tayama, H. Kimura, *Angew. Chem.-Int. Edit.*, 2007, **46**, 8869-8871.
6. G. Van Koten, J. G. Noltes, *J. Organometal. Chem.*, 1979, **174**, 367-387
7. G. M. Sheldrick, University of Gottingen, Germany, SHELXS97