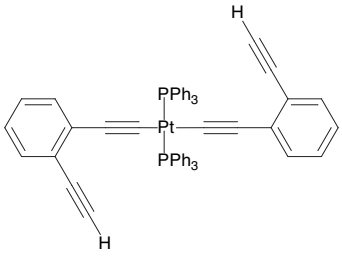
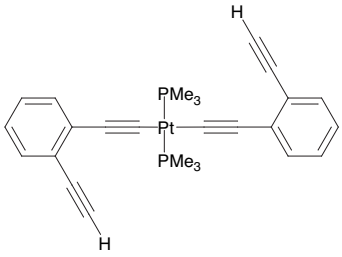
Synthesis and X-ray crystal structure of an anionic heteronuclear metallamacrocyclic triangle

José Vicente,* María-Teresa Chicote, Miguel M. Alvarez–Falcón and Peter G. Jones

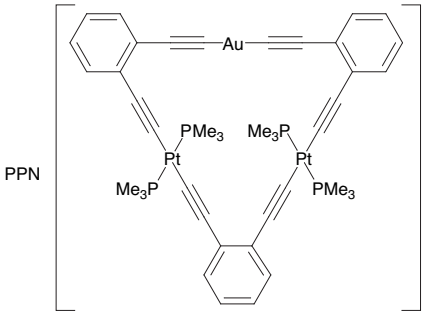
Supplementary Information

Experimental details for the preparation of





and



1 **2**

Listing of all refined and calculated atomic coordinates, anisotropic thermal parameters, and bond lengths and angles for **2**.

[Pt{C≡C(Ar)C≡CH}$_2$(PPh$_3$)$_2$] (Ar = C_6Me_4–1,2,3,4). A mixture of $C_6Me_4(C{\equiv}CH)_2$-1,2 (236 mg, 1.29 mmol) and $[PtCl_2(PPh_3)_2]$ (256 mg, 0.32 mmol) in $NHEt_2$ (20 mL) in the presence of a catalytic amount of CuI (6 mg, 0.03 mmol), was stirred under N_2 for 15 h, concentrated to dryness and the residue treated with CH_2Cl_2 (5 mL). The suspension was added dropwise to EtOH (40 mL) and filtered. The colorless solid was dried to give the complex (248 mg, 0.23 mmol, 72% yield). Mp 236 ºC (dec). Anal. Calcd. for $C_{64}H_{56}P_2Pt$: C, 71.03; H, 5.22. Found: C, 70.72; H, 5.51. IR (cm^{-1}): ν(CH), 3284(s); ν(C≡C), 2102(s). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.82 (m, 15 H, PPh_3), 7.26-7.20 (m, 15 H, PPh_3), 3.01 (s, 2 H, CH), 2.31 (s, 6 H, Me), 2.07 (s, 6 H, Me), 1.98 (s, 6 H, Me), 1.55 (s, 6 H, Me). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 135.3 (m, m-PPh_3, $^3J_{CP}$ = 5 Hz), 134.7 (Ar), 134.4 (Ar), 134.1 (Ar), 131.5 (m, i-PPh_3), 130.5 (Ar), 129.8 (m, p-PPh_3), 129.6 (Ar), 127.5 (m, o-PPh_3), 120.0 (Ar), 118.6 (CPt, $^1J_{PtC}$ = 31 Hz), 112.4 (*C*CPt, $^2J_{PtC}$ = 5 Hz), 84.3 (CH), 81.2 (*C*CH), 18.5 (Me), 17.9 (Me), 16.6 (Me), 16.4 (Me). ^{31}P{^{1}H} NMR (162 MHz, $CDCl_3$) δ 17.17 (PPh_3, $^1J_{PtP}$ = 2671 Hz). MS-FAB$^+$ (*m/z*, %) 1083 (M^+, 27%).

[Pt{C≡C(Ar)C≡CH}$_2$(PMe$_3$)$_2$] (1). To a solution of [Pt{C≡C(Ar)C≡CH}$_2$(PPh_3)$_2$] (418 mg, 0.39 mmol) in dry THF (15 mL) was added PMe_3 (1M in toluene, 2.32 mL) under N_2. The mixture was stirred for 14 h concentrated under vacuum (3 mL) and n-pentane (15 mL) added. After a few minutes, the suspension was filtered and the solid washed with n-pentane (5 mL) and dried under reduced pressure (ca. 1 mbar) to give **1** (243 mg, 0.34 mmol, 88%) as a microcrystalline colourless powder. Mp 234 ºC (dec). Anal. Calcd. for $C_{34}H_{44}P_2Pt$: C, 57.54; H, 6.25. Found: C, 57.71; H, 6.67. IR (cm^{-1}): ν(CH), 3234(s); ν(C≡C), 2084(s). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.32 (s, 2 H, CH), 2.48 (s, 6 H, Me), 2.42 (s, 6 H, Me), 2.20 (s, 6 H, Me), 2.17 (s, 6 H, Me), 1.77 (vt, 18 H, Me, PMe_3, $|^2J_{HP} + {}^4J_{HP}| = 8$ Hz, $^3J_{HPt}$ = 30 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 136.0 (Ar), 135.5 (Ar), 134.7 (Ar), 131.8 (Ar), 129.0 (Ar, $^3J_{PtC}$ = 26 Hz), 120.8 (Ar), 116.0 (*C*CPt, $^2J_{PtC}$ = 31 Hz), 106.8 (CPt, $^1J_{PtC}$

= 267 Hz), 84.8 (≡CH), 82.4 (*C*≡CH), 19.0 (Me), 18.6 (Me), 16.9 (Me), 16.5 (Me), 16.0 (vt, Me, PMe_3, $|^1J_{PC} + {}^3J_{PC}|$ = 40 Hz, $^2J_{PtC}$ = 39 Hz). $^{31}P\{^1H\}$ NMR (162 MHz, $CDCl_3$) δ -21.62 (PMe_3, $^1J_{PtP}$ = 2320 Hz). MS-FAB$^+$ (*m/z*, %) 709 (M^+, 24%).

PPN[{Au{Pt(PMe$_3$)$_2$}$_2$}{μ^2-Ar(C≡C)$_2$}$_3$] (2). To a solution of **1** (0.085 g, 0.12 mmol) in degassed CH_2Cl_2 (20 mL) was added a solution of PPN[Au(acac)$_2$] (0.134 g, 0.14 mmol) in the same solvent (5 mL) and the mixture was stirred under N_2 for 6 h, filtered through Celite and evaporated under vacuum to ca. 5 mL. The slow addition of Et_2O (20 mL) gave a fine orange suspension and a dense dark oil adhered to the flask bottom. The suspension was decanted and Et_2O (10 mL) was added to complete the precipitation of an orange solid which was filtered off and recrystallized from CH_2Cl_2 and Et_2O to give **2** (65 mg, 0.033 mmol, 55%) as a microcrystalline bright orange powder. Crystals of **2**·H_2O, suitable for an X ray diffraction study were obtained by slow diffusion of Et_2O into a solution of **2** in CH_2Cl_2. Mp 142 ºC (dec). Anal. Calcd. for $C_{90}H_{102}AuNP_6Pt_2$: C, 54.85; H, 5.22; N, 0.71. Found: C, 55.10; H, 5.06; N, 1.06. IR (cm^{-1}): ν(C≡C), 2086(s). ^1H NMR (200 MHz, $CDCl_3$) δ 7.73-7.26 (m, 30 H, PPN), 2.49 (s, 6 H, Me), 2.44 (s, 6 H, Me), 2.39 (s, 6 H, Me), 2.15 (s, 6 H, Me), 2.11 (s, 6 H, Me), 2.05 (s, 6 H, Me), 1.83 (vt, 36 H, Me, PMe_3, $|^2J_{HP} + {}^4J_{HP}|$ = 8 Hz, $^3J_{HPt}$ = 30 Hz). $^{13}C\{^1H\}$ NMR (50 MHz, $CDCl_3$) δ 142.50, 135.49, 134.89, 134.73, 134.09 (m, p-PPN), 133.82, 133.17, 131.97 (m, m-PPN), 130.81, 130.42, 130.16, 129.70 (m, o-PPN), 126.8 (dd, i-PPN, $^1J_{CP}$ = 108 Hz, $^3J_{CP}$ = 2 Hz), 123.57, 117.49, 115.26, 108.67 (C≡C), 107.95 (C≡C), 102.03 (CPt, $^1J_{CP}$ = 25 Hz), 19.27 (Me), 19.15 (Me), 19.08 (Me), 16.87 (Me), 16.68 (Me), 16.65 (Me), 16.41 (vt, Me, PMe_3, $|^1J_{PC} + {}^3J_{PC}|$ = 62 Hz). $^{31}P\{^1H\}$ NMR (81MHz, $CDCl_3$) δ 21.82 (s, PPN), -21.47 (PMe_3, $^1J_{PtP}$ = 2323 Hz). Λ_M ($\Omega^{-1}\cdot cm^2\cdot mol^{-1}$) 88. MS-FAB$^-$ (*m/z,* %) 1431 (M^-, 30%).

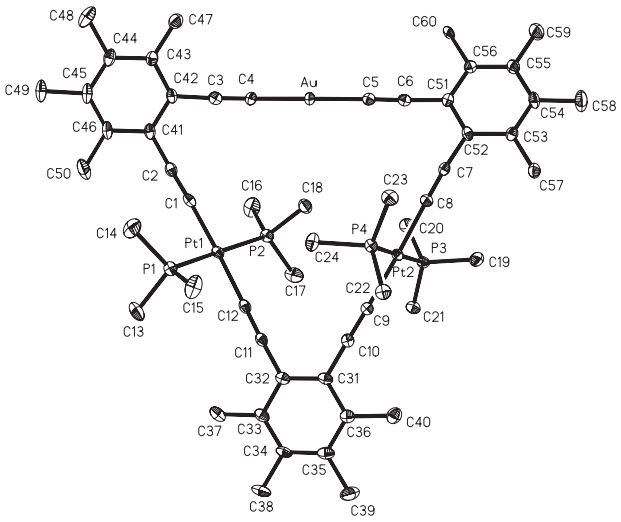


Table 1. Crystal data and structure refinement.

Identification code	mura	
Empirical formula	C90 H104 Au N O P6 Pt2	
Formula weight	1988.71	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.444(2) Å	α= 118.064(6)º
	b = 18.759(3) Å	β= 92.078(6)º
	c = 18.827(3) Å	γ = 91.734(6)º
Volume	4181.2(11) Å^3	
Z	2	
Density (calculated)	1.580 Mg/m^3	
Absorption coefficient	5.248 mm^{-1}	
F(000)	1968	
Crystal size	0.24 x 0.14 x 0.07 mm^3	
Theta range for data collection	1.23 to 28.28º	
Index ranges	-17<=h<=17, -25<=k<=25, -25<=l<=25	
Reflections collected	68098	
Independent reflections	20677 [R(int) = 0.1069]	
Completeness to theta = 28.25º	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.802 and 0.587	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20677 / 246 / 912	
Goodness-of-fit on F^2	0.956	
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.0911	
R indices (all data)	R1 = 0.0868, wR2 = 0.1094	
Largest diff. peak and hole	3.492 and -3.393 e.Å^{-3}	

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

	x	y	z	U(eq)
Au	7236.9(2)	4648.9(1)	3183.5(1)	25.5(1)
Pt(1)	8789.2(2)	7848.1(1)	5939.7(1)	25.0(1)
Pt(2)	7703.6(2)	5213.1(1)	6716.5(1)	22.6(1)
P(1)	10386.3(12)	8391.6(10)	6225.9(10)	29.1(4)
P(2)	7244.0(12)	7194.0(10)	5662.7(10)	30.5(4)
P(3)	6014.8(12)	5205.4(10)	6817.3(9)	26.0(3)
P(4)	9390.9(12)	5193.9(10)	6608.8(9)	26.2(3)
C(1)	8829(5)	7634(4)	4799(4)	28.0(13)
C(2)	8896(5)	7521(4)	4112(4)	30.0(13)
C(3)	8148(5)	6011(4)	2817(3)	28.5(13)
C(4)	7702(4)	5519(4)	2937(3)	26.0(13)
C(5)	6870(4)	3770(4)	3456(3)	26.8(13)
C(6)	6678(4)	3255(4)	3638(3)	26.1(12)
C(7)	7083(4)	3488(4)	5238(3)	25.0(12)
C(8)	7413(4)	4119(4)	5794(3)	25.4(12)
C(9)	7931(4)	6344(4)	7621(3)	24.4(12)
C(10)	8078(4)	7033(4)	8154(3)	25.9(12)
C(11)	8642(4)	8296(4)	7807(4)	27.7(13)
C(12)	8728(5)	8119(4)	7106(4)	28.7(13)
C(13)	10455(6)	9476(4)	6879(5)	51(2)
C(14)	11125(5)	8287(6)	5404(4)	53(2)
C(15)	11161(6)	8010(6)	6760(5)	55(2)
C(16)	6447(6)	7253(6)	4897(5)	58(2)
C(17)	6460(5)	7449(5)	6495(4)	51(2)
C(18)	7369(5)	6128(4)	5292(4)	40.2(16)
C(19)	5506(5)	4386(4)	6959(4)	42.6(17)
C(20)	5328(5)	5090(4)	5924(4)	36.8(16)
C(21)	5514(5)	6072(4)	7629(3)	33.7(15)
C(22)	10074(5)	5437(4)	7551(3)	31.5(14)
C(23)	9866(5)	4248(4)	5893(4)	37.3(16)
C(24)	9876(5)	5937(4)	6334(4)	39.7(17)

C(31)	8235(4)	7847(4)	8794(3)	26.9(12)
C(32)	8502(4)	8482(4)	8629(3)	27.4(12)
C(33)	8604(4)	9284(4)	9258(4)	32.0(13)
C(34)	8445(5)	9436(4)	10044(3)	32.0(14)
C(35)	8204(5)	8811(4)	10217(3)	34.9(14)
C(36)	8086(4)	8012(4)	9595(3)	29.8(13)
C(37)	8828(6)	9961(4)	9067(4)	43.0(17)
C(38)	8502(6)	10315(4)	10708(4)	48.7(19)
C(39)	8017(7)	8988(5)	11075(4)	56(2)
C(40)	7750(5)	7323(5)	9750(4)	41.8(17)
C(41)	9050(4)	7337(4)	3281(4)	31.4(13)
C(42)	8733(4)	6573(4)	2646(3)	27.6(12)
C(43)	8964(4)	6353(4)	1849(4)	30.5(13)
C(44)	9478(5)	6924(4)	1700(4)	36.0(14)
C(45)	9749(5)	7707(5)	2327(4)	42.2(16)
C(46)	9549(5)	7907(4)	3118(4)	37.6(15)
C(47)	8678(6)	5528(5)	1195(4)	44.3(17)
C(48)	9774(6)	6692(6)	849(5)	62(2)
C(49)	10305(6)	8301(5)	2136(5)	56(2)
C(50)	9833(7)	8738(5)	3797(5)	62(2)
C(51)	6420(4)	2615(4)	3824(3)	25.4(12)
C(52)	6636(4)	2733(4)	4615(3)	25.6(12)
C(53)	6365(4)	2101(4)	4804(3)	28.8(13)
C(54)	5921(5)	1369(4)	4205(4)	35.0(14)
C(55)	5739(5)	1253(4)	3415(4)	33.9(14)
C(56)	5995(5)	1876(4)	3226(3)	28.6(13)
C(57)	6579(6)	2222(4)	5639(4)	39.5(16)
C(58)	5643(7)	712(5)	4419(5)	65(3)
C(59)	5271(7)	472(5)	2773(4)	58(2)
C(60)	5792(5)	1766(4)	2392(3)	36.6(16)
P(5)	6391.8(12)	2429.3(10)	9917.1(9)	24.8(3)
P(6)	6538.2(12)	2113.3(10)	8193.2(9)	24.4(3)
N	6665(4)	2093(3)	9019(3)	28.4(11)
C(61)	5891(4)	3416(4)	10361(3)	26.3(13)
C(62)	4950(5)	3477(4)	10052(3)	31.7(14)
C(63)	4568(5)	4237(4)	10341(4)	37.5(16)

C(64)	5095(5)	4918(4)	10930(4)	37.7(15)
C(65)	6015(5)	4853(4)	11237(4)	37.0(15)
C(66)	6414(5)	4104(4)	10951(3)	30.6(14)
C(71)	7487(4)	2462(4)	10504(3)	25.7(13)
C(72)	8395(5)	2264(4)	10145(4)	31.9(14)
C(73)	9228(5)	2270(4)	10601(4)	37.8(16)
C(74)	9179(5)	2472(4)	11399(3)	32.5(14)
C(75)	8274(4)	2668(4)	11758(3)	29.1(13)
C(76)	7440(5)	2668(4)	11314(3)	27.6(13)
C(81)	5458(4)	1768(4)	10004(3)	27.0(13)
C(82)	4880(4)	2052(4)	10670(4)	31.0(14)
C(83)	4187(5)	1547(5)	10747(4)	38.3(15)
C(84)	4045(5)	761(5)	10155(4)	44.7(17)
C(85)	4609(6)	463(5)	9487(4)	45.0(17)
C(86)	5317(5)	969(4)	9407(4)	35.6(15)
C(91)	7268(4)	2926(4)	8179(3)	28.3(13)
C(92)	7203(5)	3706(4)	8824(4)	36.9(15)
C(93)	7658(5)	4357(4)	8804(4)	44.2(17)
C(94)	8186(5)	4261(4)	8155(4)	43.3(17)
C(95)	8285(6)	3489(4)	7520(4)	45.3(18)
C(96)	7824(5)	2826(4)	7530(4)	38.0(16)
C(101)	5275(5)	2222(3)	7910(3)	28.6(13)
C(102)	4513(5)	1752(4)	7984(4)	40.0(16)
C(103)	3545(6)	1795(5)	7747(5)	66(3)
C(104)	3326(7)	2317(6)	7444(7)	85(3)
C(105)	4071(6)	2790(5)	7381(6)	67(3)
C(106)	5035(5)	2746(5)	7607(4)	46.5(18)
C(111)	6905(4)	1154(4)	7421(3)	26.0(13)
C(112)	6699(5)	917(4)	6617(3)	33.2(15)
C(113)	6984(6)	184(4)	6030(4)	44.2(18)
C(114)	7497(5)	-313(4)	6249(4)	42.1(17)
C(115)	7687(5)	-94(4)	7051(4)	41.6(17)
C(116)	7408(5)	640(4)	7635(4)	32.4(14)
O(1)	6088(9)	-1273(8)	4108(7)	192(5)

Table 3. Bond lengths [Å] and angles [º].

Au-C(4)	1.987(6)	C(31)-C(32)	1.406(8)
Au-C(5)	1.997(6)	C(31)-C(36)	1.412(7)
Pt(1)-C(1)	1.994(6)	C(32)-C(33)	1.409(8)
Pt(1)-C(12)	2.013(6)	C(33)-C(34)	1.395(7)
Pt(1)-P(1)	2.2819(18)	C(33)-C(37)	1.500(9)
Pt(1)-P(2)	2.2932(18)	C(34)-C(35)	1.388(8)
Pt(2)-C(8)	1.982(6)	C(34)-C(38)	1.527(9)
Pt(2)-C(9)	2.005(6)	C(35)-C(36)	1.402(8)
Pt(2)-P(4)	2.2847(17)	C(35)-C(39)	1.520(8)
Pt(2)-P(3)	2.2854(17)	C(36)-C(40)	1.515(9)
P(1)-C(14)	1.805(7)	C(41)-C(46)	1.404(8)
P(1)-C(15)	1.805(7)	C(41)-C(42)	1.406(8)
P(1)-C(13)	1.812(7)	C(42)-C(43)	1.405(7)
P(2)-C(18)	1.797(7)	C(43)-C(44)	1.400(8)
P(2)-C(17)	1.801(7)	C(43)-C(47)	1.482(9)
P(2)-C(16)	1.813(7)	C(44)-C(45)	1.411(9)
P(3)-C(21)	1.799(6)	C(44)-C(48)	1.521(9)
P(3)-C(19)	1.800(7)	C(45)-C(46)	1.392(9)
P(3)-C(20)	1.805(6)	C(45)-C(49)	1.508(9)
P(4)-C(23)	1.803(6)	C(46)-C(50)	1.505(10)
P(4)-C(24)	1.813(6)	C(51)-C(56)	1.397(8)
P(4)-C(22)	1.814(6)	C(51)-C(52)	1.417(7)
C(1)-C(2)	1.215(8)	C(52)-C(53)	1.430(8)
C(2)-C(41)	1.459(8)	C(53)-C(54)	1.399(8)
C(3)-C(4)	1.196(9)	C(53)-C(57)	1.495(8)
C(3)-C(42)	1.457(9)	C(54)-C(55)	1.409(8)
C(5)-C(6)	1.192(8)	C(54)-C(58)	1.508(9)
C(6)-C(51)	1.437(8)	C(55)-C(56)	1.408(8)
C(7)-C(8)	1.210(8)	C(55)-C(59)	1.493(10)
C(7)-C(52)	1.442(8)	C(56)-C(60)	1.498(8)
C(9)-C(10)	1.210(8)	P(5)-N	1.564(5)
C(10)-C(31)	1.435(8)	P(5)-C(71)	1.790(6)
C(11)-C(12)	1.210(8)	P(5)-C(61)	1.800(6)
C(11)-C(32)	1.439(8)	P(5)-C(81)	1.804(7)

P(6)-N	1.577(5)	C(84)-C(85)	1.380(9)
P(6)-C(91)	1.800(7)	C(85)-C(86)	1.385(9)
P(6)-C(111)	1.800(6)	C(91)-C(96)	1.394(7)
P(6)-C(101)	1.807(6)	C(91)-C(92)	1.403(8)
C(61)-C(66)	1.390(8)	C(92)-C(93)	1.367(9)
C(61)-C(62)	1.404(7)	C(93)-C(94)	1.375(8)
C(62)-C(63)	1.387(8)	C(94)-C(95)	1.392(9)
C(63)-C(64)	1.385(9)	C(95)-C(96)	1.382(9)
C(64)-C(65)	1.379(8)	C(101)-C(102)	1.384(8)
C(65)-C(66)	1.382(8)	C(101)-C(106)	1.390(8)
C(71)-C(72)	1.392(7)	C(102)-C(103)	1.378(9)
C(71)-C(76)	1.391(7)	C(103)-C(104)	1.379(10)
C(72)-C(73)	1.384(8)	C(104)-C(105)	1.362(10)
C(73)-C(74)	1.369(8)	C(105)-C(106)	1.366(9)
C(74)-C(75)	1.387(8)	C(111)-C(112)	1.376(7)
C(75)-C(76)	1.375(7)	C(111)-C(116)	1.391(7)
C(81)-C(82)	1.387(7)	C(112)-C(113)	1.376(8)
C(81)-C(86)	1.389(8)	C(113)-C(114)	1.377(8)
C(82)-C(83)	1.367(9)	C(114)-C(115)	1.376(8)
C(83)-C(84)	1.369(9)	C(115)-C(116)	1.373(8)

C(4)-Au-C(5)	175.9(2)	C(13)-P(1)-Pt(1)	112.7(3)
C(1)-Pt(1)-C(12)	177.2(2)	C(18)-P(2)-C(17)	102.5(4)
C(1)-Pt(1)-P(1)	91.65(19)	C(18)-P(2)-C(16)	104.2(4)
C(12)-Pt(1)-P(1)	88.24(19)	C(17)-P(2)-C(16)	104.4(4)
C(1)-Pt(1)-P(2)	90.24(19)	C(18)-P(2)-Pt(1)	110.0(2)
C(12)-Pt(1)-P(2)	90.13(19)	C(17)-P(2)-Pt(1)	117.3(3)
P(1)-Pt(1)-P(2)	174.27(6)	C(16)-P(2)-Pt(1)	116.8(3)
C(8)-Pt(2)-C(9)	176.5(2)	C(21)-P(3)-C(19)	102.2(3)
C(8)-Pt(2)-P(4)	95.14(17)	C(21)-P(3)-C(20)	104.4(3)
C(9)-Pt(2)-P(4)	87.27(17)	C(19)-P(3)-C(20)	103.4(3)
C(8)-Pt(2)-P(3)	83.94(17)	C(21)-P(3)-Pt(2)	117.5(2)
C(9)-Pt(2)-P(3)	93.68(17)	C(19)-P(3)-Pt(2)	114.2(2)
P(4)-Pt(2)-P(3)	178.85(6)	C(20)-P(3)-Pt(2)	113.4(2)
C(14)-P(1)-C(15)	103.5(3)	C(23)-P(4)-C(24)	105.2(3)
C(14)-P(1)-C(13)	102.6(4)	C(23)-P(4)-C(22)	104.1(3)
C(15)-P(1)-C(13)	103.9(4)	C(24)-P(4)-C(22)	104.2(3)
C(14)-P(1)-Pt(1)	118.6(3)	C(23)-P(4)-Pt(2)	116.4(2)
C(15)-P(1)-Pt(1)	113.8(3)	C(24)-P(4)-Pt(2)	112.9(2)

C(22)-P(4)-Pt(2)	112.9(2)	C(42)-C(43)-C(47)	119.9(5)
C(2)-C(1)-Pt(1)	177.0(6)	C(43)-C(44)-C(45)	121.2(6)
C(1)-C(2)-C(41)	174.7(6)	C(43)-C(44)-C(48)	119.5(6)
C(4)-C(3)-C(42)	176.6(6)	C(45)-C(44)-C(48)	119.2(6)
C(3)-C(4)-Au	168.3(5)	C(46)-C(45)-C(44)	119.7(6)
C(6)-C(5)-Au	177.8(6)	C(46)-C(45)-C(49)	120.9(7)
C(5)-C(6)-C(51)	177.5(7)	C(44)-C(45)-C(49)	119.2(7)
C(8)-C(7)-C(52)	175.6(6)	C(45)-C(46)-C(41)	119.8(6)
C(7)-C(8)-Pt(2)	169.8(5)	C(45)-C(46)-C(50)	120.7(6)
C(10)-C(9)-Pt(2)	178.4(5)	C(41)-C(46)-C(50)	119.5(6)
C(9)-C(10)-C(31)	178.8(7)	C(56)-C(51)-C(52)	120.4(5)
C(12)-C(11)-C(32)	177.4(7)	C(56)-C(51)-C(6)	120.5(5)
C(11)-C(12)-Pt(1)	176.6(5)	C(52)-C(51)-C(6)	119.0(5)
C(32)-C(31)-C(36)	119.9(6)	C(51)-C(52)-C(53)	119.1(5)
C(32)-C(31)-C(10)	120.8(5)	C(51)-C(52)-C(7)	121.2(5)
C(36)-C(31)-C(10)	119.3(5)	C(53)-C(52)-C(7)	119.7(5)
C(31)-C(32)-C(33)	120.1(5)	C(54)-C(53)-C(52)	120.0(5)
C(31)-C(32)-C(11)	118.6(5)	C(54)-C(53)-C(57)	120.4(5)
C(33)-C(32)-C(11)	121.2(6)	C(52)-C(53)-C(57)	119.5(6)
C(34)-C(33)-C(32)	119.1(6)	C(53)-C(54)-C(55)	120.1(6)
C(34)-C(33)-C(37)	121.2(6)	C(53)-C(54)-C(58)	119.0(6)
C(32)-C(33)-C(37)	119.6(6)	C(55)-C(54)-C(58)	120.9(6)
C(35)-C(34)-C(33)	121.3(6)	C(56)-C(55)-C(54)	120.2(6)
C(35)-C(34)-C(38)	120.6(6)	C(56)-C(55)-C(59)	119.5(6)
C(33)-C(34)-C(38)	118.0(6)	C(54)-C(55)-C(59)	120.3(6)
C(34)-C(35)-C(36)	120.1(5)	C(51)-C(56)-C(55)	120.2(5)
C(34)-C(35)-C(39)	120.6(6)	C(51)-C(56)-C(60)	119.0(5)
C(36)-C(35)-C(39)	119.2(6)	C(55)-C(56)-C(60)	120.8(6)
C(35)-C(36)-C(31)	119.5(6)	N-P(5)-C(71)	108.4(3)
C(35)-C(36)-C(40)	121.7(5)	N-P(5)-C(61)	115.1(3)
C(31)-C(36)-C(40)	118.7(6)	C(71)-P(5)-C(61)	108.8(3)
C(46)-C(41)-C(42)	120.1(6)	N-P(5)-C(81)	110.4(3)
C(46)-C(41)-C(2)	120.2(6)	C(71)-P(5)-C(81)	108.1(3)
C(42)-C(41)-C(2)	119.7(5)	C(61)-P(5)-C(81)	105.8(3)
C(43)-C(42)-C(41)	120.7(5)	N-P(6)-C(91)	113.0(3)
C(43)-C(42)-C(3)	119.8(6)	N-P(6)-C(111)	107.0(2)
C(41)-C(42)-C(3)	119.5(5)	C(91)-P(6)-C(111)	110.2(3)
C(44)-C(43)-C(42)	118.4(6)	N-P(6)-C(101)	114.7(3)
C(44)-C(43)-C(47)	121.7(6)	C(91)-P(6)-C(101)	105.5(3)

C(111)-P(6)-C(101)	106.4(3)	C(85)-C(86)-C(81)	119.7(6)
P(5)-N-P(6)	149.2(3)	C(96)-C(91)-C(92)	119.0(6)
C(66)-C(61)-C(62)	120.3(5)	C(96)-C(91)-P(6)	123.0(5)
C(66)-C(61)-P(5)	122.9(4)	C(92)-C(91)-P(6)	117.8(5)
C(62)-C(61)-P(5)	116.7(4)	C(93)-C(92)-C(91)	120.2(6)
C(63)-C(62)-C(61)	118.4(6)	C(92)-C(93)-C(94)	120.9(6)
C(64)-C(63)-C(62)	120.9(6)	C(93)-C(94)-C(95)	119.8(7)
C(65)-C(64)-C(63)	120.4(6)	C(96)-C(95)-C(94)	119.9(6)
C(64)-C(65)-C(66)	119.7(6)	C(95)-C(96)-C(91)	120.2(6)
C(65)-C(66)-C(61)	120.3(6)	C(102)-C(101)-C(106)	118.3(6)
C(72)-C(71)-C(76)	119.3(5)	C(102)-C(101)-P(6)	118.8(4)
C(72)-C(71)-P(5)	119.9(4)	C(106)-C(101)-P(6)	122.9(5)
C(76)-C(71)-P(5)	120.8(4)	C(103)-C(102)-C(101)	120.6(6)
C(73)-C(72)-C(71)	119.1(5)	C(102)-C(103)-C(104)	120.0(8)
C(74)-C(73)-C(72)	121.4(6)	C(105)-C(104)-C(103)	119.7(8)
C(73)-C(74)-C(75)	119.6(6)	C(104)-C(105)-C(106)	120.7(7)
C(76)-C(75)-C(74)	119.7(5)	C(105)-C(106)-C(101)	120.6(7)
C(75)-C(76)-C(71)	120.8(5)	C(112)-C(111)-C(116)	119.1(6)
C(82)-C(81)-C(86)	119.5(6)	C(112)-C(111)-P(6)	121.2(4)
C(82)-C(81)-P(5)	120.3(5)	C(116)-C(111)-P(6)	119.8(4)
C(86)-C(81)-P(5)	120.2(5)	C(111)-C(112)-C(113)	120.8(6)
C(83)-C(82)-C(81)	120.5(6)	C(114)-C(113)-C(112)	119.6(6)
C(82)-C(83)-C(84)	119.9(6)	C(115)-C(114)-C(113)	120.3(6)
C(83)-C(84)-C(85)	120.8(7)	C(116)-C(115)-C(114)	120.0(6)
C(84)-C(85)-C(86)	119.6(7)	C(115)-C(116)-C(111)	120.2(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$). 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	25.5(1)	25.4(1)	29.0(1)	15.9(1)	0.6(1)	-0.6(1)
Pt(1)	21.8(1)	20.7(1)	28.9(1)	8.8(1)	0.3(1)	2.1(1)
Pt(2)	21.2(1)	21.1(1)	24.1(1)	9.7(1)	-1.6(1)	0.2(1)
P(1)	23.8(9)	28.6(9)	34.9(8)	15.1(7)	0.8(7)	2.6(7)
P(2)	24.1(9)	31.0(9)	33.6(8)	13.1(7)	0.2(7)	1.9(7)
P(3)	23.7(8)	27.2(9)	24.3(7)	9.9(6)	-0.3(6)	0.4(7)
P(4)	22.4(8)	25.0(8)	30.3(8)	12.3(7)	0.9(7)	1.4(7)
C(1)	24(3)	19(3)	37(3)	10(3)	-5(3)	0(3)
C(2)	24(3)	27(3)	39(3)	16(3)	-2(3)	-1(3)
C(3)	25(3)	31(3)	30(3)	14(3)	-5(3)	4(3)
C(4)	21(3)	31(3)	30(3)	18(3)	1(3)	1(3)
C(5)	20(3)	29(3)	29(3)	12(3)	4(3)	4(3)
C(6)	23(3)	27(3)	26(3)	11(2)	-2(2)	3(3)
C(7)	20(3)	31(3)	28(3)	18(2)	1(2)	0(2)
C(8)	23(3)	25(3)	27(3)	11(2)	2(2)	3(2)
C(9)	20(3)	27(3)	27(3)	13(2)	1(2)	2(3)
C(10)	20(3)	28(3)	31(3)	15(2)	-1(3)	2(3)
C(11)	18(3)	26(3)	35(3)	11(3)	2(3)	-3(3)
C(12)	26(3)	21(3)	37(3)	12(3)	3(3)	3(3)
C(13)	39(5)	31(4)	71(5)	13(4)	5(4)	-8(3)
C(14)	23(4)	86(7)	56(5)	38(5)	4(4)	-6(4)
C(15)	32(4)	82(7)	81(6)	62(5)	6(4)	12(4)
C(16)	32(4)	83(7)	70(5)	48(5)	-14(4)	-8(4)
C(17)	27(4)	57(5)	51(4)	9(4)	5(3)	0(4)
C(18)	43(4)	30(4)	44(4)	14(3)	5(3)	-1(3)
C(19)	45(5)	46(5)	37(3)	20(3)	8(3)	-4(4)
C(20)	31(4)	44(4)	36(3)	20(3)	-9(3)	0(3)
C(21)	30(4)	32(4)	33(3)	10(3)	0(3)	3(3)
C(22)	22(3)	37(4)	35(3)	17(3)	2(3)	5(3)
C(23)	26(4)	38(4)	44(4)	14(3)	10(3)	8(3)
C(24)	34(4)	46(4)	52(4)	33(4)	8(3)	4(3)
C(31)	15(3)	31(3)	26(3)	7(2)	-5(2)	-1(3)
C(32)	18(3)	29(3)	29(3)	8(2)	-1(2)	3(3)
C(33)	21(3)	29(3)	36(3)	8(2)	-2(3)	-1(3)

C(34)	24(3)	30(3)	26(3)	1(2)	-6(3)	-1(3)
C(35)	23(3)	45(4)	27(3)	10(3)	-6(3)	1(3)
C(36)	20(3)	36(3)	31(3)	14(2)	-5(3)	1(3)
C(37)	45(5)	27(3)	46(4)	9(3)	-7(3)	-3(3)
C(38)	48(5)	40(4)	31(3)	-5(3)	-6(3)	-4(4)
C(39)	72(6)	61(6)	30(3)	17(3)	5(4)	9(5)
C(40)	39(4)	51(4)	43(4)	28(3)	-1(3)	2(3)
C(41)	32(4)	28(3)	45(3)	26(3)	-1(3)	3(3)
C(42)	22(3)	27(3)	38(3)	20(2)	-2(3)	-1(3)
C(43)	22(3)	36(3)	38(3)	22(3)	1(3)	1(3)
C(44)	27(4)	50(4)	48(3)	37(3)	0(3)	1(3)
C(45)	29(4)	49(4)	70(4)	47(3)	-2(3)	-6(3)
C(46)	33(4)	36(4)	57(4)	34(3)	-1(3)	-6(3)
C(47)	46(5)	52(4)	35(3)	22(3)	0(3)	-9(4)
C(48)	51(5)	101(7)	61(4)	61(5)	12(4)	9(5)
C(49)	53(5)	57(5)	86(6)	56(5)	5(5)	-9(4)
C(50)	73(6)	41(4)	79(5)	35(4)	-15(5)	-21(4)
C(51)	20(3)	31(3)	30(3)	18(2)	1(2)	2(2)
C(52)	16(3)	25(3)	37(3)	15(2)	1(2)	-2(2)
C(53)	23(3)	34(3)	33(3)	19(3)	3(3)	-1(3)
C(54)	33(4)	29(3)	47(3)	23(3)	-7(3)	-11(3)
C(55)	32(4)	32(3)	36(3)	15(3)	-4(3)	-8(3)
C(56)	28(3)	30(3)	28(3)	14(2)	1(3)	2(3)
C(57)	54(5)	32(4)	37(3)	21(3)	-5(3)	-6(3)
C(58)	85(7)	54(5)	70(5)	45(5)	-25(5)	-30(5)
C(59)	79(6)	42(4)	47(4)	19(3)	-11(4)	-20(4)
C(60)	50(4)	21(3)	29(3)	6(3)	-10(3)	-21(3)
P(5)	24.0(8)	28.2(9)	26.1(7)	16.1(7)	-0.2(6)	3.4(7)
P(6)	26.0(8)	26.5(8)	26.4(7)	17.1(6)	0.4(6)	4.1(7)
C(61)	28(3)	27(3)	31(3)	19(2)	1(3)	5(3)
C(62)	32(4)	31(3)	33(3)	16(3)	0(3)	3(3)
C(63)	32(4)	44(4)	42(4)	24(3)	-2(3)	13(3)
C(64)	49(4)	32(3)	39(3)	22(3)	10(3)	13(3)
C(65)	46(4)	31(3)	37(3)	19(3)	2(3)	4(3)
C(66)	36(4)	31(3)	31(3)	19(3)	-1(3)	3(3)
C(71)	25(3)	27(3)	29(3)	16(3)	-3(2)	1(3)
C(72)	31(4)	34(4)	30(3)	15(3)	2(3)	2(3)
C(73)	23(3)	44(4)	44(3)	18(3)	6(3)	8(3)
C(74)	24(3)	30(4)	38(3)	12(3)	-9(3)	1(3)

C(75)	27(3)	31(3)	30(3)	15(3)	-3(2)	4(3)
C(76)	27(3)	30(3)	29(3)	16(3)	4(3)	7(3)
C(81)	25(3)	30(3)	30(3)	18(3)	-5(2)	4(3)
C(82)	24(3)	39(4)	33(3)	21(3)	-1(3)	4(3)
C(83)	24(4)	56(4)	49(4)	36(3)	2(3)	7(3)
C(84)	27(4)	60(5)	64(4)	46(4)	-14(3)	-11(3)
C(85)	55(5)	37(4)	46(4)	25(3)	-18(3)	-11(3)
C(86)	46(4)	31(3)	35(3)	20(3)	-6(3)	0(3)
C(91)	28(3)	29(3)	32(3)	18(3)	-1(3)	2(3)
C(92)	44(4)	30(4)	39(3)	18(3)	9(3)	2(3)
C(93)	50(5)	28(4)	47(4)	11(3)	3(3)	-1(3)
C(94)	43(4)	41(4)	58(4)	34(3)	0(4)	-8(3)
C(95)	53(5)	45(4)	43(4)	25(3)	8(4)	-9(4)
C(96)	42(4)	38(4)	37(3)	20(3)	4(3)	-5(3)
C(101)	26(3)	26(3)	34(3)	15(3)	-2(3)	2(3)
C(102)	37(4)	40(4)	51(4)	28(3)	1(3)	2(3)
C(103)	30(4)	76(7)	112(7)	61(6)	-5(5)	-8(4)
C(104)	42(5)	99(9)	154(10)	92(8)	-8(6)	8(5)
C(105)	49(5)	58(6)	119(7)	64(6)	-15(5)	9(4)
C(106)	43(4)	49(5)	65(5)	42(4)	-2(4)	8(4)
C(111)	23(3)	27(3)	31(3)	17(3)	-1(3)	0(3)
C(112)	43(4)	30(3)	32(3)	19(3)	-1(3)	2(3)
C(113)	66(5)	28(4)	36(3)	15(3)	-6(3)	-3(4)
C(114)	49(5)	22(3)	47(3)	10(3)	2(3)	6(3)
C(115)	37(4)	39(4)	49(4)	21(3)	-6(3)	11(3)
C(116)	35(4)	25(3)	43(3)	21(3)	-5(3)	4(3)

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

	x	y	z	U(eq)
H(13A)	10064	9603	7349	62
H(13B)	10186	9746	6583	62
H(13C)	11151	9665	7057	62
H(14A)	10759	8481	5074	64
H(14B)	11261	7717	5071	64
H(14C)	11756	8608	5620	64
H(15A)	10815	8040	7222	67
H(15B)	11790	8336	6951	67
H(15C)	11297	7445	6398	67
H(16A)	6339	7822	5055	69
H(16B)	5805	6965	4841	69
H(16C)	6766	7005	4381	69
H(17A)	6346	8029	6751	62
H(17B)	6787	7319	6891	62
H(17C)	5820	7139	6298	62
H(18A)	7789	5921	4829	48
H(18B)	6709	5846	5125	48
H(18C)	7677	6035	5719	48
H(19A)	5835	4399	7438	51
H(19B)	5615	3870	6485	51
H(19C)	4789	4442	7031	51
H(20A)	5557	5515	5796	44
H(20B)	4616	5133	6020	44
H(20C)	5439	4559	5472	44
H(21A)	5751	6564	7614	40
H(21B)	5735	6103	8145	40
H(21C)	4785	6022	7570	40
H(22A)	9860	5949	7977	38
H(22B)	10789	5486	7489	38
H(22C)	9942	5005	7694	38
H(23A)	9532	4071	5361	45
H(23B)	9740	3839	6067	45
H(23C)	10585	4322	5862	45
H(24A)	9642	6470	6701	48

H(24B)	9642	5786	5779	48
H(24C)	10606	5958	6372	48
H(37A)	8244	10287	9158	65
H(37B)	8994	9737	8502	65
H(37C)	9394	10303	9417	65
H(38A)	8447	10331	11233	73
H(38B)	7955	10601	10616	73
H(38C)	9141	10577	10701	73
H(39A)	7388	9256	11233	84
H(39B)	8564	9343	11441	84
H(39C)	7979	8480	11104	84
H(40A)	8030	7419	10278	63
H(40B)	7982	6814	9330	63
H(40C)	7020	7289	9744	63
H(47A)	8157	5557	834	67
H(47B)	8426	5193	1429	67
H(47C)	9262	5286	891	67
H(48A)	10443	6485	776	92
H(48B)	9771	7169	764	92
H(48C)	9297	6273	459	92
H(49A)	10570	8764	2639	85
H(49B)	9850	8488	1848	85
H(49C)	10856	8036	1798	85
H(50A)	10552	8783	3930	94
H(50B)	9470	8827	4272	94
H(50C)	9662	9145	3633	94
H(57A)	5950	2219	5885	59
H(57B)	6949	2742	5962	59
H(57C)	6978	1784	5617	59
H(58A)	6194	350	4309	97
H(58B)	5045	402	4095	97
H(58C)	5511	956	4992	97
H(59A)	4746	581	2468	87
H(59B)	4981	163	3021	87
H(59C)	5778	158	2408	87
H(60A)	5786	2297	2411	55
H(60B)	5143	1476	2174	55
H(60C)	6314	1453	2046	55
H(62)	4583	3009	9654	38

H(63)	3937	4290	10132	45
H(64)	4820	5433	11124	45
H(65)	6373	5321	11642	44
H(66)	7050	4058	11159	37
H(72)	8442	2127	9594	38
H(73)	9847	2130	10356	45
H(74)	9761	2479	11704	39
H(75)	8232	2801	12309	35
H(76)	6823	2810	11564	33
H(82)	4967	2600	11075	37
H(83)	3805	1742	11210	46
H(84)	3551	417	10205	54
H(85)	4513	-86	9085	54
H(86)	5703	770	8946	43
H(92)	6842	3782	9277	44
H(93)	7609	4883	9243	53
H(94)	8481	4720	8140	52
H(95)	8670	3418	7080	54
H(96)	7886	2300	7094	46
H(102)	4659	1397	8199	48
H(103)	3028	1465	7793	79
H(104)	2659	2346	7279	103
H(105)	3918	3154	7178	80
H(106)	5546	3078	7557	56
H(112)	6355	1264	6466	40
H(113)	6828	21	5477	53
H(114)	7720	-809	5846	50
H(115)	8012	-451	7199	50
H(116)	7558	798	8188	39