

Supporting Information

Coordination-Driven Assembly of Molecular Rectangles via an Organometallic "Clip"

Christopher J. Kuehl, Charles L. Mayne, Atta M. Arif, and Peter J. Stang*

Department of Chemistry, University of Utah, 315 S. 1400 E., Salt Lake City, Utah 84112, USA

stang@chemistry.utah.edu

1,8-Bis(*trans*-Pt(PEt₃)₂Cl)anthracene. To a stirred solution of Pt(PEt₃)₄ (2 g, 0.003 mol) in freshly distilled toluene (60 mL) under argon, was added, in portions, 1,8-dichloroanthracene (336 mg, 1.36 mmol). The resulting bright red solution was then heated overnight (18 h) in an oil bath maintained at 105-110°C. The following day the solvent was removed in vacuo, and the residue, now in open air, was suspended in methanol (15 mL) and gently refluxed for 45 minutes. The suspension was then allowed to cool, the product collected on a frit, and washed twice with cold methanol (5 mL each) to give **1** as a yellow solid. A 1.3 g quantity (86% yield) was obtained. mp 262-268 °C (dec.). ¹H NMR (CD₂Cl₂, 300 MHz): δ 9.33 (s, 1H, H⁹), 8.15 (s, 1H, H¹⁰), 7.56 (m, 4H, H^{2,4,5,7}), 6.98 (m, 2H, H^{3,6}), 1.67 (m, 24H, PCH₂CH₃), 0.93 (m, 36H, PCH₂CH₃). ³¹P{¹H} NMR (CD₂Cl₂, 121.4 MHz): δ 10.7 (s, ¹J_{Pt} = 2756 Hz). ¹³C{¹H} NMR (CD₂Cl₂, 125.7 MHz): δ 142.3 (m, ¹J_{C_{Pt}} = 973 Hz, C_i-Pt), 138.9, 135.8, 133.2, 131.9, 126.3, 125.8, 122.0, 14.8 (m, PCH₂CH₃), 8.3 (s, PCH₂CH₃). Anal. Calcd for C₃₈H₆₈Cl₂P₄Pt₂: C, 41.12; H, 6.18. Found: C, 41.19; H, 6.24.

1,8-Bis(*trans*-Pt(PEt₃)₂(NO₃))anthracene (1**).** To a stirred solution of 1,8-Bis(*trans*-Pt(PEt₃)₂Cl)anthracene (500 mg, 0.450 mmol) in acetone (60 mL), was added, all at once, silver

nitrate (153 mg, 0.900 mmol). The reaction was stirred for 3 h in the dark, after which the reaction mixture was filtered through a bed of celite and the filtrate evaporated to dryness under reduced pressure. The crude yellow solid was then suspended in 20 mL of water and sonicated for 15 minutes. The suspension was then filtered, washed with excess water, and air dried. Next, on a steam bath, the product was taken up in a minimum amount of boiling ethanol, filtered hot, and placed in the freezer for 1-2 days. The yellow crystals that formed were collected on a frit and dried in vacuo to give 430 mg (82% yield) of analytically pure product. mp 257-258 °C (dec.). ^1H NMR (acetone- d_6 , 300 MHz): δ 9.54 (s, 1H, H^9), 8.24 (s, 1H, H^{10}), 7.67 (m, 4H, $\text{H}^{2,4,5,7}$), 7.05 (m, 2H, $\text{H}^{3,6}$), 1.63 (m, 24H, PCH_2CH_3), 1.03 (m, 36H, PCH_2CH_3). $^{31}\text{P}\{^1\text{H}\}$ NMR (acetone- d_6 , 121.4 MHz): δ 14.6 (s, $^1J_{\text{PPt}} = 2855$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (acetone- d_6 , 125.7 MHz): δ 138.4, 133.4, 132.6, 130.1, 127.6, 127.5, 125.9, 123.5, 15.3 (m, PCH_2CH_3), 8.0 (s, PCH_2CH_3). Anal. Calcd for $\text{C}_{38}\text{H}_{68}\text{N}_2\text{O}_6\text{P}_4\text{Pt}_2$: C, 39.24; H, 5.89; N, 2.41. Found: C, 39.50; H, 5.92; N, 2.38.

Cyclobis[(1,8-Bis(*trans*-Pt(PEt_3) $_2$ (NO_3))anthracene)(4,4'-dipyridyl)] (2a). In a 2 dram vial equipped with a magnetic stir bar, were placed solid 1,8-Bis(*trans*-Pt(PEt_3) $_2$ (NO_3))anthracene (21.3 mg, 0.018 mmol) and 4,4'-dipyridyl (2.9 mg, 0.018 mmol). Next, 0.6 mL of acetone- d_6 and 0.6 mL of D_2O were added to the vial which was then sealed with teflon tape and heated in an oil bath at 50-55 °C, with stirring. After 2 h the initial pale yellow suspension gradually turned bright orange and became homogeneous. The orange solution was then transferred to an NMR tube for analysis. The product was precipitated with KPF_6 , collected on a frit, washed with excess water, and dried in vacuo. ^1H NMR (acetone- $d_6/\text{D}_2\text{O}$, 300 MHz): δ 9.60 (s, 2H, H^9), 9.28 (d, 4H, $^1J_{\text{HH}} = 6.3$ Hz, $\text{H}_\alpha\text{-Py}$), 9.22 (d, 4H, $^1J_{\text{HH}} = 5.7$ Hz, $\text{H}_\alpha\text{-Py}$), 8.88 (d, 4H, $^1J_{\text{HH}} = 6.0$ Hz, $\text{H}_\beta\text{-Py}$), 8.63 (d, 4H, $^1J_{\text{HH}} = 6.3$ Hz, $\text{H}_\beta\text{-Py}$), 8.43 (s, 2H, H^{10}), 7.77 (d, 4H, $^1J_{\text{HH}} = 8.4$ Hz, $\text{H}^{4,5}$),

7.70 (d, 4H, $^1J_{\text{HH}} = 6.9$ Hz, $\text{H}^{2,7}$), 7.20 (m, 4H, $\text{H}^{3,6}$), 1.54 (m, 48H, PCH_2CH_3), 0.88 (m, 72H, PCH_2CH_3). $^{31}\text{P}\{^1\text{H}\}$ NMR (acetone- d_6 /D $_2$ O, 121.4 MHz): δ 8.6 (s, $^1J_{\text{PPt}} = 2647$ Hz).

Cyclobis[(1,8-Bis(*trans*-Pt(P Et_3) $_2$ (NO $_3$))anthracene)(4,4''-dipyridyl-1',4'-diethynylbenzene)]

(2b). In a 2 dram vial equipped with a magnetic stir bar, were placed solid 1,8-Bis(*trans*-Pt(P Et_3) $_2$ (NO $_3$))anthracene (17.8 mg, 0.015 mmol) and 4,4''-dipyridyl-1',4'-diethynylbenzene, (4.3 mg, 0.015 mmol). Next, 0.6 ml of acetone- d_6 and 0.6 mL of D $_2$ O were added to the vial which was then sealed with teflon tape and heated in an oil bath at 50-55 °C, with stirring. After 2 h the initial pale yellow suspension gradually turned bright orange and became homogeneous. The orange solution was then transferred to an NMR tube for analysis. The product was precipitated with KPF $_6$, collected on a frit, washed with excess water, and dried in vacuo. ^1H NMR (acetone- d_6 /D $_2$ O, 300 MHz): δ 9.45 (s, 2H, H^9), 9.05 (d, 4H, $^1J_{\text{HH}} = 5.4$ Hz, $\text{H}_{\alpha\text{-Py}}$), 8.96 (d, 4H, $^1J_{\text{HH}} = 6.3$ Hz, $\text{H}_{\alpha\text{-Py}}$), 8.36 (s, 2H, H^{10}), 8.05 (d, 8H, $^1J_{\text{HH}} = 6.3$ Hz, $\text{H}_{\beta\text{-Py}}$), 7.76 (s, 8H, $\text{H}_{\text{phenylene}}$), 7.71 (d, 4H, $^1J_{\text{HH}} = 8.1$ Hz, $\text{H}^{4,5}$), 7.64 (d, 4H, $^1J_{\text{HH}} = 6.6$ Hz, $\text{H}^{2,7}$), 7.16 (m, 4H, $\text{H}^{3,6}$), 1.44 (m, 48H, PCH_2CH_3), 0.82 (m, 72H, PCH_2CH_3). $^{31}\text{P}\{^1\text{H}\}$ NMR (acetone- d_6 /D $_2$ O, 121.4 MHz): δ 8.4 (s, $^1J_{\text{PPt}} = 2643$ Hz).

Table 1. Crystal data and structure refinement for shelxl.

Identification code	shelxl	
Empirical formula	C102 H161 F24 N7 P12 Pt4	
Formula weight	3093.38	
Temperature	200(0.1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P 2_1/c$	
Unit cell dimensions	$a = 20.0273(4)$ Å	$\alpha = 90^\circ$.
	$b = 15.2535(2)$ Å	$\beta = 112.7372(7)^\circ$.
	$c = 21.7461(5)$ Å	$\gamma = 90^\circ$.
Volume	$6126.9(2)$ Å ³	
Z	2	
Density (calculated)	1.677 Mg/m ³	
Absorption coefficient	4.791 mm ⁻¹	
F(000)	3060	
Crystal size	0.30 x 0.25 x 0.13 mm ³	
Theta range for data collection	2.32 to 32.58°.	
Index ranges	$-30 \leq h \leq 30$, $-18 \leq k \leq 18$, $-32 \leq l \leq 32$	
Reflections collected	34298	
Independent reflections	20145 [R(int) = 0.0416]	
Completeness to theta = 32.58°	90.3 %	
Absorption correction	SCALEPACK	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	20145 / 6 / 683	
Goodness-of-fit on F ²	1.057	
Final R indices [I > 2sigma(I)]	R1 = 0.0611, wR2 = 0.1409	
R indices (all data)	R1 = 0.1041, wR2 = 0.1672	
Largest diff. peak and hole	2.400 and -2.299 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for shelxl. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Pt(1)	-1865(1)	-415(1)	6950(1)	41(1)
Pt(2)	3411(1)	351(1)	11407(1)	42(1)
P(1)	-1754(1)	-1930(2)	7034(1)	61(1)
P(2)	-1981(1)	1061(2)	6675(2)	70(1)
P(3)	3509(1)	-1164(2)	11451(1)	64(1)
P(4)	3505(1)	1846(1)	11277(1)	50(1)
P(5)	3293(2)	-599(2)	8505(2)	100(1)
P(6)	386(3)	7273(2)	4972(3)	138(2)
F(1)	3477(6)	101(5)	9066(5)	144(4)
F(2)	3017(5)	-1221(5)	8938(5)	136(3)
F(3)	4053(7)	-1061(7)	8797(6)	187(5)
F(4)	3564(6)	25(5)	8087(5)	153(4)
F(5)	2500(6)	-199(8)	8187(5)	161(4)
F(6)	3081(6)	-1312(5)	7932(5)	160(4)
F(7)	942(6)	7967(7)	5268(5)	184(5)
F(8)	-87(7)	7963(10)	4517(10)	286(10)
F(9)	832(14)	7079(10)	4506(14)	366(14)
F(10)	894(8)	6576(9)	5477(11)	268(9)
F(11)	12(10)	7332(10)	5388(9)	269(9)
F(12)	-63(13)	6480(9)	4666(10)	310(11)
N(1)	-825(3)	-209(4)	7719(3)	49(1)
N(2)	2478(3)	261(4)	10497(3)	48(1)
C(1)	-2865(3)	-587(4)	6228(3)	40(1)
C(2)	-2901(4)	-669(5)	5582(4)	53(2)
C(3)	-3565(4)	-775(5)	5036(3)	54(2)
C(4)	-4192(4)	-849(5)	5128(3)	51(2)
C(5)	-4193(3)	-780(4)	5780(3)	43(2)
C(6)	-3521(3)	-629(4)	6347(3)	36(1)
C(7)	-4836(3)	-832(5)	5873(3)	46(2)
C(8)	-3568(3)	-544(4)	6980(3)	38(1)
C(9)	4277(4)	475(4)	12286(3)	45(2)

C(10)	4953(4)	506(5)	12267(4)	54(2)
C(11)	5590(4)	640(6)	12835(4)	56(2)
C(12)	5549(4)	759(5)	13432(4)	51(2)
C(13)	4874(3)	727(5)	13499(3)	45(2)
C(14)	4218(3)	583(4)	12928(3)	39(1)
C(15)	-197(4)	-318(6)	7652(4)	60(2)
C(16)	470(4)	-203(6)	8170(4)	57(2)
C(17)	506(3)	43(5)	8782(3)	43(1)
C(18)	-155(4)	215(7)	8831(4)	73(3)
C(19)	-783(4)	87(8)	8296(4)	74(3)
C(20)	1190(3)	141(5)	9373(3)	43(1)
C(21)	1862(4)	77(6)	9332(3)	53(2)
C(22)	2489(4)	144(6)	9900(4)	55(2)
C(23)	1827(4)	332(6)	10536(4)	63(2)
C(24)	1190(4)	283(6)	10002(4)	64(2)
C(25)	-1013(8)	-2329(8)	7747(7)	130(6)
C(26)	-911(11)	-3343(10)	7751(10)	197(10)
C(27)	-2546(7)	-2511(8)	7091(7)	97(4)
C(28)	-3116(9)	-2810(8)	6492(8)	132(6)
C(29)	-1691(10)	-2409(10)	6307(7)	145(7)
C(30)	-1002(9)	-2015(13)	6175(10)	163(8)
C(31)	-1357(6)	1792(7)	7280(7)	102(4)
C(32)	-1278(8)	2709(9)	7056(9)	146(6)
C(33)	-2862(6)	1576(7)	6509(7)	104(4)
C(34)	-3412(7)	1611(9)	5845(8)	143(7)
C(35)	-1817(8)	1221(9)	5930(7)	115(5)
C(36)	-1114(10)	813(13)	5972(8)	156(7)
C(37)	3449(11)	-1631(15)	12254(11)	110(9)
C(37)	4226(17)	-1687(18)	12119(15)	140(19)
C(38)	4176(7)	-1801(11)	12784(8)	136(6)
C(39)	2758(15)	-1750(17)	11120(50)	230(50)
C(39)	2610(30)	-1766(19)	11100(40)	410(80)
C(40)	2780(12)	-2757(10)	11009(17)	320(20)
C(41)	4339(10)	-1517(14)	11404(9)	94(8)
C(41)	3730(20)	-1594(17)	10707(12)	109(13)
C(42)	4407(15)	-1218(14)	10737(11)	190(10)

C(43)	3796(5)	2519(5)	12031(4)	58(2)
C(44)	3820(6)	3504(6)	11932(5)	81(3)
C(45)	2700(5)	2393(6)	10695(5)	72(2)
C(46)	2111(6)	2515(8)	10962(6)	95(4)
C(47)	4195(5)	2060(6)	10953(4)	65(2)
C(48)	4091(7)	1593(10)	10307(6)	109(4)
N(3)	2235(10)	4815(12)	630(10)	176(7)
C(49)	2068(14)	5051(18)	995(14)	183(9)
C(50)	1900(20)	5590(20)	1550(20)	330(20)
N(4)	600(20)	5530(20)	1600(20)	188(14)
C(51)	450(60)	5170(70)	1090(30)	410(60)
C(52)	270(30)	4940(40)	351(19)	220(20)

Table 3. Bond lengths [Å] and angles [°] for shelxl.

Pt(1)-C(1)	2.028(6)
Pt(1)-N(1)	2.132(5)
Pt(1)-P(2)	2.318(2)
Pt(1)-P(1)	2.321(2)
Pt(2)-C(9)	2.034(6)
Pt(2)-N(2)	2.138(6)
Pt(2)-P(4)	2.314(2)
Pt(2)-P(3)	2.318(2)
P(1)-C(25)	1.788(11)
P(1)-C(29)	1.792(13)
P(1)-C(27)	1.862(12)
P(2)-C(35)	1.790(15)
P(2)-C(31)	1.807(10)
P(2)-C(33)	1.836(11)
P(3)-C(39)	1.65(3)
P(3)-C(41)	1.787(19)
P(3)-C(37')	1.79(2)
P(3)-C(39')	1.91(6)
P(3)-C(37)	1.93(2)
P(3)-C(41')	1.95(3)
P(4)-C(47)	1.809(9)
P(4)-C(45)	1.823(9)
P(4)-C(43)	1.828(8)
P(5)-F(4)	1.553(7)
P(5)-F(1)	1.554(8)
P(5)-F(3)	1.572(11)
P(5)-F(2)	1.578(7)
P(5)-F(6)	1.583(8)
P(5)-F(5)	1.588(11)
P(6)-F(11)	1.381(11)
P(6)-F(7)	1.490(10)
P(6)-F(12)	1.501(12)
P(6)-F(8)	1.503(13)
P(6)-F(10)	1.583(15)

P(6)-F(9)	1.616(15)
N(1)-C(19)	1.305(10)
N(1)-C(15)	1.330(9)
N(2)-C(22)	1.320(9)
N(2)-C(23)	1.343(10)
C(1)-C(2)	1.384(10)
C(1)-C(6)	1.435(9)
C(2)-C(3)	1.410(10)
C(3)-C(4)	1.351(11)
C(4)-C(5)	1.423(10)
C(5)-C(7)	1.380(10)
C(5)-C(6)	1.449(8)
C(6)-C(8)	1.421(9)
C(7)-C(13)#1	1.407(10)
C(8)-C(14)#1	1.392(9)
C(9)-C(10)	1.372(10)
C(9)-C(14)	1.456(10)
C(10)-C(11)	1.405(10)
C(11)-C(12)	1.343(11)
C(12)-C(13)	1.415(10)
C(13)-C(7)#1	1.407(10)
C(13)-C(14)	1.434(8)
C(14)-C(8)#1	1.392(9)
C(15)-C(16)	1.387(10)
C(16)-C(17)	1.358(10)
C(17)-C(18)	1.393(10)
C(17)-C(20)	1.481(9)
C(18)-C(19)	1.359(11)
C(20)-C(24)	1.385(10)
C(20)-C(21)	1.386(9)
C(21)-C(22)	1.384(9)
C(23)-C(24)	1.355(10)
C(25)-C(26)	1.560(18)
C(27)-C(28)	1.435(17)
C(29)-C(30)	1.63(2)
C(31)-C(32)	1.510(16)

C(33)-C(34)	1.438(17)
C(35)-C(36)	1.51(2)
C(37)-C(38)	1.490(16)
C(37)-C(38)	1.50(4)
C(39)-C(40)	1.559(18)
C(39)-C(40)	1.579(19)
C(41)-C(42)	1.576(17)
C(41)-C(42)	1.45(4)
C(43)-C(44)	1.522(12)
C(45)-C(46)	1.514(14)
C(47)-C(48)	1.515(13)
N(3)-C(49)	1.04(3)
C(49)-C(50)	1.60(4)
N(4)-C(51)	1.17(2)
C(51)-C(52)	1.551(19)

C(1)-Pt(1)-N(1)	178.6(3)
C(1)-Pt(1)-P(2)	87.4(2)
N(1)-Pt(1)-P(2)	91.67(19)
C(1)-Pt(1)-P(1)	88.19(19)
N(1)-Pt(1)-P(1)	92.87(18)
P(2)-Pt(1)-P(1)	169.74(10)
C(9)-Pt(2)-N(2)	177.6(3)
C(9)-Pt(2)-P(4)	86.74(19)
N(2)-Pt(2)-P(4)	91.92(17)
C(9)-Pt(2)-P(3)	91.50(19)
N(2)-Pt(2)-P(3)	90.21(17)
P(4)-Pt(2)-P(3)	167.85(9)
C(25)-P(1)-C(29)	107.9(7)
C(25)-P(1)-C(27)	102.9(7)
C(29)-P(1)-C(27)	102.5(8)
C(25)-P(1)-Pt(1)	115.5(4)
C(29)-P(1)-Pt(1)	112.0(6)
C(27)-P(1)-Pt(1)	114.9(4)
C(35)-P(2)-C(31)	104.9(7)
C(35)-P(2)-C(33)	105.2(7)

C(31)-P(2)-C(33)	102.7(6)
C(35)-P(2)-Pt(1)	109.3(5)
C(31)-P(2)-Pt(1)	116.1(4)
C(33)-P(2)-Pt(1)	117.4(4)
C(39)-P(3)-C(41)	121.6(18)
C(39)-P(3)-C(37')	115(2)
C(41)-P(3)-C(37')	55.9(15)
C(39)-P(3)-C(39')	5(3)
C(41)-P(3)-C(39')	126.2(19)
C(37')-P(3)-C(39')	117(2)
C(39)-P(3)-C(37)	80(4)
C(41)-P(3)-C(37)	108.9(9)
C(37')-P(3)-C(37)	54.0(15)
C(39')-P(3)-C(37)	79(3)
C(39)-P(3)-C(41')	85(3)
C(41)-P(3)-C(41')	48.5(13)
C(37')-P(3)-C(41')	99.0(18)
C(39')-P(3)-C(41')	89(3)
C(37)-P(3)-C(41')	137.7(12)
C(39)-P(3)-Pt(2)	118.2(9)
C(41)-P(3)-Pt(2)	111.3(7)
C(37')-P(3)-Pt(2)	120.5(9)
C(39')-P(3)-Pt(2)	114.3(9)
C(37)-P(3)-Pt(2)	111.7(8)
C(41')-P(3)-Pt(2)	110.2(9)
C(47)-P(4)-C(45)	104.5(4)
C(47)-P(4)-C(43)	102.8(4)
C(45)-P(4)-C(43)	104.8(4)
C(47)-P(4)-Pt(2)	109.6(3)
C(45)-P(4)-Pt(2)	116.4(3)
C(43)-P(4)-Pt(2)	117.2(3)
F(4)-P(5)-F(1)	90.4(5)
F(4)-P(5)-F(3)	90.5(6)
F(1)-P(5)-F(3)	95.2(7)
F(4)-P(5)-F(2)	179.0(4)
F(1)-P(5)-F(2)	88.7(4)

F(3)-P(5)-F(2)	89.9(6)
F(4)-P(5)-F(6)	90.5(5)
F(1)-P(5)-F(6)	178.3(6)
F(3)-P(5)-F(6)	86.2(6)
F(2)-P(5)-F(6)	90.4(5)
F(4)-P(5)-F(5)	91.5(6)
F(1)-P(5)-F(5)	88.4(6)
F(3)-P(5)-F(5)	175.9(7)
F(2)-P(5)-F(5)	88.2(5)
F(6)-P(5)-F(5)	90.2(6)
F(11)-P(6)-F(7)	100.2(10)
F(11)-P(6)-F(12)	87.6(9)
F(7)-P(6)-F(12)	169.6(11)
F(11)-P(6)-F(8)	91.3(11)
F(7)-P(6)-F(8)	87.9(7)
F(12)-P(6)-F(8)	98.9(12)
F(11)-P(6)-F(10)	87.5(10)
F(7)-P(6)-F(10)	90.3(8)
F(12)-P(6)-F(10)	83.1(10)
F(8)-P(6)-F(10)	177.6(12)
F(11)-P(6)-F(9)	173.0(9)
F(7)-P(6)-F(9)	84.2(9)
F(12)-P(6)-F(9)	87.4(10)
F(8)-P(6)-F(9)	94.3(13)
F(10)-P(6)-F(9)	87.0(11)
C(19)-N(1)-C(15)	115.9(6)
C(19)-N(1)-Pt(1)	119.0(5)
C(15)-N(1)-Pt(1)	125.0(5)
C(22)-N(2)-C(23)	117.4(6)
C(22)-N(2)-Pt(2)	125.3(5)
C(23)-N(2)-Pt(2)	117.3(5)
C(2)-C(1)-C(6)	119.1(6)
C(2)-C(1)-Pt(1)	116.4(5)
C(6)-C(1)-Pt(1)	124.4(5)
C(1)-C(2)-C(3)	121.9(7)
C(4)-C(3)-C(2)	120.9(7)

C(3)-C(4)-C(5)	120.0(6)
C(7)-C(5)-C(4)	120.1(6)
C(7)-C(5)-C(6)	119.8(6)
C(4)-C(5)-C(6)	120.1(6)
C(8)-C(6)-C(1)	125.3(5)
C(8)-C(6)-C(5)	116.8(6)
C(1)-C(6)-C(5)	117.9(6)
C(5)-C(7)-C(13)#1	122.7(6)
C(14)#1-C(8)-C(6)	123.3(5)
C(10)-C(9)-C(14)	118.2(6)
C(10)-C(9)-Pt(2)	117.9(5)
C(14)-C(9)-Pt(2)	123.7(5)
C(9)-C(10)-C(11)	123.3(7)
C(12)-C(11)-C(10)	119.7(7)
C(11)-C(12)-C(13)	120.8(6)
C(7)#1-C(13)-C(12)	120.6(6)
C(7)#1-C(13)-C(14)	118.7(6)
C(12)-C(13)-C(14)	120.6(6)
C(8)#1-C(14)-C(13)	118.6(6)
C(8)#1-C(14)-C(9)	124.1(5)
C(13)-C(14)-C(9)	117.3(6)
N(1)-C(15)-C(16)	123.4(7)
C(17)-C(16)-C(15)	120.0(7)
C(16)-C(17)-C(18)	115.9(6)
C(16)-C(17)-C(20)	124.0(6)
C(18)-C(17)-C(20)	120.1(6)
C(19)-C(18)-C(17)	120.0(8)
N(1)-C(19)-C(18)	124.5(8)
C(24)-C(20)-C(21)	116.5(6)
C(24)-C(20)-C(17)	121.3(6)
C(21)-C(20)-C(17)	122.2(6)
C(22)-C(21)-C(20)	120.3(7)
N(2)-C(22)-C(21)	122.3(7)
N(2)-C(23)-C(24)	123.7(7)
C(23)-C(24)-C(20)	119.7(7)
C(26)-C(25)-P(1)	113.9(10)

C(28)-C(27)-P(1)	119.3(10)
C(30)-C(29)-P(1)	111.0(10)
C(32)-C(31)-P(2)	117.8(10)
C(34)-C(33)-P(2)	121.2(11)
C(36)-C(35)-P(2)	112.5(10)
C(38)-C(37)-P(3)	112.4(15)
C(38)-C(37')-P(3)	120(3)
C(37)-C(38)-C(37')	69.0(17)
C(40)-C(39)-P(3)	121.6(17)
C(40)-C(39')-P(3)	107(3)
C(39)-C(40)-C(39')	11(3)
C(42)-C(41)-P(3)	112.2(13)
C(42)-C(41')-P(3)	109.7(16)
C(41')-C(42)-C(41)	61.0(14)
C(44)-C(43)-P(4)	116.4(6)
C(46)-C(45)-P(4)	113.6(7)
C(48)-C(47)-P(4)	115.1(7)
N(3)-C(49)-C(50)	168(3)
N(4)-C(51)-C(52)	164(10)

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	31(1)	53(1)	32(1)	-3(1)	4(1)	1(1)
Pt(2)	35(1)	52(1)	30(1)	-4(1)	3(1)	-1(1)
P(1)	58(1)	55(1)	48(1)	-6(1)	-3(1)	12(1)
P(2)	48(1)	55(1)	93(2)	10(1)	12(1)	-9(1)
P(3)	51(1)	53(1)	61(1)	-3(1)	-7(1)	9(1)
P(4)	49(1)	55(1)	38(1)	1(1)	8(1)	-4(1)
P(5)	155(3)	63(2)	134(3)	-24(2)	114(3)	-18(2)
P(6)	119(3)	68(2)	244(6)	13(3)	88(4)	-14(2)
F(1)	248(11)	93(5)	155(7)	-40(5)	149(8)	-40(6)
F(2)	215(9)	82(4)	173(8)	-6(5)	140(7)	-18(5)
F(3)	208(11)	179(10)	248(13)	14(9)	168(11)	53(8)
F(4)	263(11)	91(5)	197(9)	-8(5)	189(9)	-22(6)
F(5)	176(9)	230(11)	110(7)	18(7)	92(7)	51(8)
F(6)	248(11)	109(6)	181(9)	-71(6)	149(9)	-48(6)
F(7)	179(9)	166(9)	164(9)	28(7)	19(7)	-76(8)
F(8)	155(10)	194(13)	390(20)	121(14)	-31(12)	-24(9)
F(9)	520(30)	180(13)	640(40)	-57(19)	490(30)	-76(17)
F(10)	215(13)	150(10)	520(30)	115(14)	235(17)	23(10)
F(11)	410(20)	210(13)	350(20)	14(13)	320(20)	47(14)
F(12)	460(30)	157(10)	440(30)	-116(13)	320(20)	-192(15)
N(1)	31(3)	69(4)	37(3)	-11(3)	2(2)	-1(2)
N(2)	41(3)	60(4)	35(3)	-5(2)	5(2)	-3(3)
C(1)	29(3)	46(3)	34(3)	-2(2)	-1(2)	0(2)
C(2)	49(4)	59(4)	40(4)	0(3)	7(3)	4(3)
C(3)	58(4)	59(4)	31(3)	0(3)	3(3)	7(3)
C(4)	54(4)	49(4)	30(3)	-2(3)	-4(3)	3(3)
C(5)	39(3)	38(3)	34(3)	0(2)	-6(2)	4(2)
C(6)	32(3)	33(3)	32(3)	0(2)	-1(2)	2(2)
C(7)	32(3)	52(4)	33(3)	-4(3)	-10(2)	0(3)
C(8)	31(3)	40(3)	29(3)	1(2)	-4(2)	-2(2)
C(9)	40(3)	43(4)	34(3)	-3(3)	-3(2)	-3(3)

C(10)	37(3)	70(5)	48(4)	-4(3)	6(3)	1(3)
C(11)	28(3)	76(5)	51(4)	-8(4)	2(3)	-2(3)
C(12)	31(3)	62(4)	43(4)	-7(3)	-2(3)	-6(3)
C(13)	36(3)	45(4)	41(3)	-3(3)	-2(3)	-1(3)
C(14)	32(3)	39(3)	34(3)	-1(2)	0(2)	-2(2)
C(15)	39(4)	98(6)	33(3)	-13(4)	4(3)	4(4)
C(16)	31(3)	92(6)	39(3)	-10(4)	3(3)	1(3)
C(17)	30(3)	54(4)	36(3)	-5(3)	3(2)	-2(3)
C(18)	42(4)	131(8)	40(4)	-10(5)	11(3)	4(5)
C(19)	39(4)	128(8)	48(4)	-9(5)	10(3)	6(5)
C(20)	31(3)	53(4)	38(3)	-5(3)	7(2)	-2(3)
C(21)	38(3)	86(5)	30(3)	-11(3)	7(3)	3(3)
C(22)	32(3)	82(5)	39(3)	-18(3)	2(3)	-3(3)
C(23)	41(4)	102(7)	39(4)	-10(4)	7(3)	-8(4)
C(24)	37(4)	114(7)	34(3)	-11(4)	7(3)	-8(4)
C(25)	143(12)	82(8)	98(9)	-3(7)	-29(8)	41(8)
C(26)	200(20)	98(11)	197(19)	22(12)	-24(15)	70(12)
C(27)	108(9)	76(7)	112(10)	7(7)	47(8)	5(6)
C(28)	139(13)	73(8)	152(14)	-18(8)	21(11)	-17(8)
C(29)	189(17)	116(11)	86(9)	-53(8)	3(10)	45(11)
C(30)	121(12)	212(19)	195(18)	-57(15)	105(13)	10(13)
C(31)	76(7)	57(6)	135(10)	-9(6)	-3(7)	-21(5)
C(32)	114(11)	83(9)	202(17)	-1(10)	19(11)	-41(8)
C(33)	66(7)	60(6)	172(13)	15(7)	33(8)	6(5)
C(34)	77(8)	84(8)	193(16)	4(9)	-30(9)	18(6)
C(35)	108(10)	98(9)	132(12)	34(8)	38(9)	-16(8)
C(36)	138(14)	230(20)	127(13)	1(13)	77(12)	-68(14)
C(37)	89(16)	89(15)	124(19)	14(13)	12(14)	-10(12)
C(37)	120(20)	84(17)	110(20)	62(16)	-71(19)	-47(16)
C(38)	100(10)	152(14)	162(15)	65(12)	56(10)	25(9)
C(39)	24(10)	34(17)	520(130)	-10(30)	-20(20)	10(9)
C(39)	300(70)	50(20)	480(120)	-10(30)	-270(80)	-20(30)
C(40)	156(19)	75(11)	570(60)	-50(20)	-50(30)	7(11)
C(41)	69(12)	102(15)	85(15)	-22(11)	0(10)	20(10)
C(41)	190(40)	66(15)	56(13)	-29(11)	37(19)	13(18)
C(42)	250(30)	180(20)	190(20)	-30(16)	140(20)	49(19)

C(43)	65(5)	56(4)	42(4)	-5(3)	11(3)	-2(4)
C(44)	85(7)	56(5)	82(7)	-1(5)	11(5)	1(5)
C(45)	60(5)	75(6)	60(5)	12(4)	0(4)	-4(4)
C(46)	58(6)	96(8)	117(9)	18(7)	18(6)	12(5)
C(47)	59(5)	77(6)	52(4)	6(4)	15(4)	-8(4)
C(48)	119(10)	158(12)	76(7)	-18(7)	65(8)	-30(9)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for shelxl.

	x	y	z	U(eq)
H(2)	-2465	-653	5505	63
H(3)	-3572	-795	4597	64
H(4)	-4633	-947	4757	61
H(7)	-5269	-944	5497	55
H(8)	-3133	-457	7360	46
H(10)	4994	433	11849	65
H(11)	6047	647	12797	67
H(12)	5979	865	13813	61
H(15)	-207	-484	7228	72
H(16)	903	-295	8097	69
H(18)	-165	422	9239	87
H(19)	-1223	223	8344	88
H(21)	1892	-14	8911	64
H(22)	2943	106	9859	66
H(23)	1812	422	10963	76
H(24)	745	345	10059	76
H(25A)	-563	-2043	7765	156
H(25B)	-1090	-2158	8154	156
H(26A)	-494	-3514	8151	296
H(26B)	-828	-3519	7353	296
H(26C)	-1348	-3634	7751	296
H(27A)	-2359	-3027	7383	117
H(27B)	-2766	-2116	7322	117
H(28A)	-3491	-3097	6604	198
H(28B)	-2919	-3228	6263	198
H(28C)	-3325	-2308	6199	198
H(29A)	-1638	-3053	6365	174
H(29B)	-2141	-2290	5915	174
H(30A)	-976	-2291	5777	244
H(30B)	-555	-2137	6561	244

H(30C)	-1060	-1380	6106	244
H(31A)	-1509	1839	7662	123
H(31B)	-873	1513	7448	123
H(32A)	-922	3033	7429	219
H(32B)	-1746	3010	6908	219
H(32C)	-1113	2680	6687	219
H(33A)	-3077	1274	6792	124
H(33B)	-2766	2188	6672	124
H(34A)	-3842	1907	5855	214
H(34B)	-3541	1013	5675	214
H(34C)	-3228	1935	5554	214
H(35A)	-2221	961	5549	139
H(35B)	-1805	1857	5846	139
H(36A)	-1052	911	5552	234
H(36B)	-1124	182	6052	234
H(36C)	-710	1082	6339	234
H(37A)	3185	-1210	12423	132
H(37B)	3170	-2185	12146	132
H(37C)	4291	-2278	11961	168
H(37D)	4675	-1354	12193	168
H(38A)	4119	-2030	13182	205
H(38B)	4453	-1253	12896	205
H(38C)	4435	-2231	12624	205
H(39A)	2484	-1663	11413	273
H(39B)	2467	-1485	10687	273
H(39C)	2350	-1718	11404	487
H(39D)	2294	-1512	10660	487
H(40A)	2287	-2971	10760	487
H(40B)	2985	-3057	11440	487
H(40C)	3080	-2875	10754	487
H(41A)	4750	-1274	11788	113
H(41B)	4368	-2164	11436	113
H(41C)	3766	-2241	10727	130
H(41D)	3334	-1430	10281	130
H(42A)	4863	-1437	10728	284
H(42B)	4401	-576	10713	284

H(42C)	4000	-1455	10356	284
H(43A)	3466	2403	12263	69
H(43B)	4286	2324	12330	69
H(44A)	3983	3799	12366	121
H(44B)	3336	3714	11650	121
H(44C)	4157	3635	11716	121
H(45A)	2841	2974	10582	86
H(45B)	2503	2045	10278	86
H(46A)	1695	2810	10625	143
H(46B)	2297	2872	11367	143
H(46C)	1961	1941	11066	143
H(47A)	4212	2699	10881	78
H(47B)	4670	1886	11294	78
H(48A)	4488	1745	10170	164
H(48B)	3629	1774	9960	164
H(48C)	4087	958	10374	164
H(50A)	2169	5331	1989	499
H(50B)	1384	5577	1451	499
H(50C)	2060	6202	1551	499
H(52A)	-259	4935	110	326
H(52B)	464	4360	319	326
H(52C)	483	5380	155	326
