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Crystal structural analysis

Crystals were used as supplied. A prism of dimensions  $0.14 \times 0.15 \times 0.36$  mm was mounted on a fiber and protected with a coating of epoxy resin. The orientation parameters and cell dimensions were obtained from the setting angles of an Enraf-Nonius CAD-4 diffractometer for 25 centered reflections in the range  $14^\circ \leq \theta \leq 15^\circ$ . Table 1 contains a summary of crystal data and the final residuals. A more extensive table including particulars of data collection and structure refinement is in the supplementary material. Absorption corrections based on azimuthal ( $\psi$ ) scans were applied. The systematic absences unambiguously indicated the space-group Pbca. The platinum atom was located from the Patterson function. A cycle of DIRDIF<sup>1</sup> gave the positions of most of the other non-hydrogen atoms. One ethyl group [C(41,42)] attached to P(2) refined with large thermal parameters and unusual bond lengths and angles; there were no clear indications of alternative positions for these atoms, and a satisfactory convergence could be obtained only when they were constrained with isotropic thermal parameters at the positions indicated by a difference synthesis. Hydrogen atoms were included at calculated positions with  $B(H) = 1.2B_{eq}(C)$  and updated after each cycle of refinement. The TEXSAN program suite,<sup>2</sup> incorporating complex atomic scattering factors,<sup>3</sup> was used in all calculations.

References

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2. Molecular Structures Corporation, 3200A Research Forest Drive, The Woodlands, TX 77381, USA. *TEXSAN: Texray Program for Structure Analysis*, version 5.0, 1989.
3. Cromer, D.T.; Waber, J.T. In *International Tables for X-Ray Crystallography*, vol. IV (eds. Ibers, J.A.; Hamilton, W.T.), 1974, pp. 71, 148. Kynoch Press, Birmingham, England.

**Table 1****Crystallographic data**

<b>Composition</b>	<b>C<sub>42</sub>H<sub>42</sub>P<sub>2</sub>Pt</b>	<b>d<sub>calc</sub></b>	<b>1.441 g cm<sup>-3</sup></b>
<b>Formula wt</b>	<b>803.83</b>	<b>T</b>	<b>22 °C</b>
<b>Space-group</b>	<b>Pbca</b>	<b>λ</b>	<b>0.71073 Å</b>
<b>a</b>	<b>14.446(2) Å</b>	<b>μ</b>	<b>39.4 cm<sup>-1</sup></b>
<b>b</b>	<b>17.184(3) Å</b>	<b>Rel trans coefft</b>	<b>0.921-1.000 (<math>\psi</math>)</b>
<b>c</b>	<b>29.856(3) Å</b>	<b>No. obs. rflns</b>	<b>3772 [<math>I \geq 1.5\sigma(I)</math>]</b>
<b>V</b>	<b>7411(3) Å<sup>3</sup></b>	<b>R(F<sub>o</sub>)</b>	<b>0.050</b>
<b>Z</b>	<b>8</b>	<b>wR(F<sub>o</sub>)</b>	<b>0.045</b>

$$R(F) = \frac{\sum |F_o - F_c|}{\sum |F_o|}$$

$$wR(F) = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{\frac{1}{2}}$$

Table 2

Atomic coordinates and equivalent isotropic thermal parameters ( $\text{\AA}^2$ )

$$B_{\text{eq}} = (8\pi^2/3) \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

Atom	x	y	z	$B_{\text{eq}}$
Pt	0.19020(3)	0.52607(2)	0.612442(12)	3.99(2)
P(1)	0.15632(19)	0.61871(16)	0.56014(9)	4.0(1)
P(2)	0.2237(3)	0.4279(2)	0.66100(12)	7.4(2)
C(1)	0.2069(7)	0.4530(6)	0.5611(3)	4.2(5)
C(2)	0.2307(7)	0.4139(6)	0.5300(4)	4.4(6)
C(3)	0.2640(8)	0.3720(6)	0.4908(3)	4.2(6)
C(4)	0.2008(8)	0.3394(7)	0.4611(4)	5.3(6)
C(5)	0.2317(9)	0.3001(7)	0.4237(4)	6.5(8)
C(6)	0.3262(8)	0.2930(7)	0.4144(3)	5.8(7)
C(7)	0.3868(7)	0.3267(6)	0.4434(3)	4.3(5)
C(8)	0.3582(7)	0.3636(6)	0.4820(3)	3.9(5)
C(9)	0.4237(7)	0.3956(6)	0.5125(3)	4.2(6)
C(10)	0.4843(8)	0.4185(6)	0.5370(3)	4.7(6)
C(11)	0.5567(8)	0.4423(6)	0.5644(3)	4.8(6)
C(12)	0.6174(8)	0.4638(7)	0.5870(4)	4.8(6)
C(13)	0.6957(8)	0.4869(6)	0.6121(3)	4.5(5)
C(14)	0.7863(9)	0.4617(8)	0.5991(4)	6.6(8)
C(15)	0.8643(9)	0.4817(9)	0.6219(4)	7.5(8)
C(16)	0.8581(8)	0.5287(9)	0.6581(5)	7.6(8)
C(17)	0.7726(10)	0.5563(8)	0.6720(4)	7.2(8)

C(18)	0.6903 (8)	0.5350 (6)	0.6498 (3)	4.6 (5)
C(19)	0.6062 (8)	0.5657 (7)	0.6650 (4)	5.0 (6)
C(20)	0.5390 (8)	0.5960 (7)	0.6806 (4)	4.8 (6)
C(21)	0.4636 (8)	0.6319 (7)	0.7012 (4)	4.8 (6)
C(22)	0.4001 (8)	0.6635 (7)	0.7203 (3)	4.6 (6)
C(23)	0.3301 (7)	0.7015 (6)	0.7443 (3)	3.8 (5)
C(24)	0.3517 (8)	0.7477 (7)	0.7811 (4)	5.5 (6)
C(25)	0.2842 (11)	0.7860 (7)	0.8043 (4)	6.3 (8)
C(26)	0.1910 (11)	0.7778 (7)	0.7917 (4)	6.1 (7)
C(27)	0.1663 (8)	0.7313 (6)	0.7556 (3)	4.9 (6)
C(28)	0.2355 (8)	0.6929 (6)	0.7315 (3)	4.0 (5)
C(29)	0.2116 (7)	0.6452 (6)	0.6940 (3)	4.1 (6)
C(30)	0.1963 (8)	0.6014 (6)	0.6630 (3)	4.7 (6)
C(31)	0.0659 (7)	0.5851 (6)	0.5221 (3)	4.5 (5)
C(32)	0.0387 (8)	0.6407 (7)	0.4855 (4)	6.4 (7)
C(33)	0.2552 (9)	0.6385 (7)	0.5236 (4)	6.1 (7)
C(34)	0.3385 (8)	0.6676 (9)	0.5480 (5)	9 (1)
C(35)	0.1197 (8)	0.7121 (6)	0.5809 (3)	5.2 (6)
C(36)	0.0293 (9)	0.7099 (7)	0.6059 (4)	7.5 (8)
C(37)	0.1790 (13)	0.3317 (8)	0.6445 (4)	9 (1)
C(38)	0.0804 (13)	0.3267 (10)	0.6363 (5)	10 (1)
C(39)	0.1914 (19)	0.4408 (11)	0.7185 (5)	16 (2)
C(40)	0.0971 (17)	0.4568 (14)	0.7254 (7)	14 (2)
C(41) <sup>a</sup>	0.3494	0.3892	0.6564	12.0
C(42) <sup>a</sup>	0.3909	0.4240	0.6586	15.0

<sup>a</sup>Isotropic; parameters not refined

**Table 3****Bond lengths (Å)**

Pt-P(1)	2.283(3)	C(13)-C(18)	1.398(13)
Pt-P(2)	2.277(4)	C(14)-C(15)	1.361(16)
Pt-C(1)	2.00(1)	C(15)-C(16)	1.350(16)
Pt-C(30)	1.996(10)	C(16)-C(17)	1.387(16)
P(1)-C(31)	1.826(9)	C(17)-C(18)	1.410(14)
P(1)-C(33)	1.829(12)	C(18)-C(19)	1.400(14)
P(1)-C(35)	1.801(11)	C(19)-C(20)	1.196(14)
P(2)-C(37)	1.841(16)	C(20)-C(21)	1.394(15)
P(2)-C(39)	1.794(17)	C(21)-C(22)	1.210(14)
P(2)-C(41)	1.94 <sup>a</sup>	C(22)-C(23)	1.402(14)
C(1)-C(2)	1.198(12)	C(23)-C(24)	1.390(13)
C(2)-C(3)	1.456(13)	C(23)-C(28)	1.427(13)
C(3)-C(4)	1.388(13)	C(24)-C(25)	1.367(15)
C(3)-C(8)	1.394(13)	C(25)-C(26)	1.405(16)
C(4)-C(5)	1.379(14)	C(26)-C(27)	1.386(15)
C(5)-C(6)	1.399(15)	C(27)-C(28)	1.399(13)
C(6)-C(7)	1.362(13)	C(28)-C(29)	1.429(13)
C(7)-C(8)	1.378(12)	C(29)-C(30)	1.213(13)
C(8)-C(9)	1.424(13)	C(31)-C(32)	1.530(13)
C(9)-C(10)	1.207(13)	C(33)-C(34)	1.492(16)
C(10)-C(11)	1.389(14)	C(35)-C(36)	1.504(15)
C(11)-C(12)	1.166(13)	C(37)-C(38)	1.448(20)

C(12)-C(13) 1.415(14) C(39)-C(40) 1.405(31)

C(13)-C(14) 1.432(14) C(41)-C(42) 0.85<sup>a</sup>

(a) C(41,42) not refined

Table 4

## Bond angles (°)

P(1)-Pt-P(2)	176.3(1)	C(11)-C(12)-C(13)	176(1)
P(1)-Pt-C(1)	86.5(3)	C(12)-C(13)-C(14)	120(1)
P(1)-Pt-C(30)	94.3(3)	C(12)-C(13)-C(18)	123(1)
P(2)-Pt-C(1)	89.8(3)	C(14)-C(13)-C(18)	117(1)
P(2)-Pt-C(30)	89.4(3)	C(13)-C(14)-C(15)	123(1)
C(1)-Pt-C(30)	170.4(4)	C(14)-C(15)-C(16)	120(1)
Pt-P(1)-C(31)	111.0(3)	C(15)-C(16)-C(17)	120(1)
Pt-P(1)-C(33)	111.7(4)	C(16)-C(17)-C(18)	121(1)
Pt-P(1)-C(35)	116.6(4)	C(13)-C(18)-C(17)	119(1)
C(31)-P(1)-C(33)	104.3(5)	C(13)-C(18)-C(19)	122(1)
C(31)-P(1)-C(35)	106.7(5)	C(17)-C(18)-C(19)	119(1)
C(33)-P(1)-C(35)	105.6(5)	C(18)-C(19)-C(20)	174(1)
Pt-P(2)-C(37)	114.8(5)	C(19)-C(20)-C(21)	177(1)
Pt-P(2)-C(39)	117.6(6)	C(20)-C(21)-C(22)	178(1)
Pt-P(2)-C(41)	114 <sup>a</sup>	C(21)-C(22)-C(23)	177(1)
C(37)-P(2)-C(39)	106.0(9)	C(22)-C(23)-C(24)	121(1)
C(37)-P(2)-C(41)	90 <sup>a</sup>	C(22)-C(23)-C(28)	120.3(9)
C(39)-P(2)-C(41)	111 <sup>a</sup>	C(24)-C(23)-C(28)	119(1)
Pt-C(1)-C(2)	169.7(9)	C(23)-C(24)-C(25)	121(1)
C(1)-C(2)-C(3)	175(1)	C(24)-C(25)-C(26)	120(1)
C(2)-C(3)-C(4)	120(1)	C(25)-C(26)-C(27)	121(1)
C(2)-C(3)-C(8)	122(1)	C(26)-C(27)-C(28)	119(1)

C(4)-C(3)-C(8)	119(1)	C(23)-C(28)-C(27)	119.8(9)
C(3)-C(4)-C(5)	120(1)	C(23)-C(28)-C(29)	120(1)
C(4)-C(5)-C(6)	121(1)	C(27)-C(28)-C(29)	120(1)
C(5)-C(6)-C(7)	118(1)	C(28)-C(29)-C(30)	175(1)
C(6)-C(7)-C(8)	122(1)	Pt-C(30)-C(29)	172(1)
C(3)-C(8)-C(7)	120(1)	P(1)-C(31)-C(32)	115.9(8)
C(3)-C(8)-C(9)	119(1)	P(1)-C(33)-C(34)	113.7(8)
C(7)-C(8)-C(9)	121(1)	P(1)-C(35)-C(36)	113.8(8)
C(8)-C(9)-C(10)	175(1)	P(2)-C(37)-C(38)	116(1)
C(9)-C(10)-C(11)	177(1)	P(2)-C(39)-C(40)	115(2)
C(10)-C(11)-C(12)	179(1)	P(2)-C(41)-C(42)	115 <sup>a</sup>

<sup>a</sup>C(41,42) not refined

Supplementary material

## Crystallographic information

Crystal data

Formula	C <sub>42</sub> H <sub>42</sub> P <sub>2</sub> Pt
Formula weight	803.83
Crystal system	orthorhombic
Space-group	Pbca
a, b, c	14.446(2), 17.184(3), 29.856(3) Å
V	7411(3) Å <sup>3</sup>
Z	8
d <sub>calc</sub>	1.441 g cm <sup>-3</sup>
μ	39.4 cm <sup>-1</sup>
F <sub>000</sub>	3216

Data collection

Crystal appearance	pale yellow prism
Crystal dimensions	0.14 × 0.15 × 0.36 mm
Diffractometer	Enraf-Nonius CAD-4
Radiation, wavelength	Mo Kα, 0.71073 Å
Monochromator	graphite
Temperature	22 °C
2θ <sub>max</sub>	50°
Index range h, k, l	0→17, 0→20, 0→35
Scan mode	ω scans

Scan speed (on  $\omega$ )  $1.0\text{--}4.1^\circ \text{ min}^{-1}$   
 Scan width  $(0.90 + 0.35\tan\theta)^\circ$   
 Reference reflections 3, every 3600 s exposure  
 No. indep. rflns scanned 6510 (excluding syst. absences)  
 $R_{\text{int}}$  no equiv. rflns measured

Refinement

Absorption correction Azimuthal scans  
 Rel. transmission factors 0.921-1.000  
 Sec. extinction parameter (g) predicted neg., fixed at zero  
 No. rflns in refinement (N) 3772 [ $I \geq 1.5\sigma(I)$ ]  
 No. parameters (V) 388  
 Function minimized  $\sum w(|F_o| - |F_c|)^2$   
 Weighting factor w  $1/\sigma^2(F)$   
 $R(F)$ ,  $wR(F)$  0.050, 0.045  
 S 1.69  
 Max.  $\Delta/\sigma$ , last cycle 0.06  
 Max., min. in final diff. map  $+0.96, -1.23 \text{ e } \text{\AA}^{-3}$

$$R(F) = \sum ||F_o| - |F_c|| / \sum |F_o| \quad wR(F) = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2}$$

$$S = [\sum w(|F_o| - |F_c|)^2 / (N-V)]^{1/2} \quad I_o(\text{corr}) = I_o(1+2gI_c)$$

Supplementary materialCalculated coordinates and thermal parameters ( $\text{\AA}^2$ ) for hydrogen atoms

Atom	x	y	z	B
H(1)	0.1363	0.3443	0.4666	6.4
H(2)	0.1879	0.2775	0.4039	7.8
H(3)	0.3473	0.2655	0.3887	6.9
H(4)	0.4511	0.3247	0.4369	5.2
H(5)	0.7922	0.4295	0.5734	8.0
H(6)	0.9228	0.4627	0.6125	9.0
H(7)	0.9125	0.5429	0.6740	9.1
H(8)	0.7695	0.5903	0.6970	8.7
H(9)	0.4145	0.7528	0.7902	6.6
H(10)	0.3002	0.8181	0.8291	7.6
H(11)	0.1443	0.8044	0.8080	7.3
H(12)	0.1031	0.7257	0.7474	5.8
H(13)	0.0870	0.5384	0.5084	5.4
H(14)	0.0122	0.5743	0.5394	5.4
H(15)	0.0914	0.6527	0.4678	7.7
H(16)	-0.0074	0.6174	0.4672	7.7
H(17)	0.0149	0.6871	0.4984	7.7
H(18)	0.2714	0.5917	0.5086	7.3
H(19)	0.2373	0.6766	0.5023	7.3
H(20)	0.3597	0.6288	0.5682	11.2
H(21)	0.3860	0.6794	0.5270	11.2

H(22)	0.3228	0.7133	0.5642	<b>11.2</b>
H(23)	0.1661	0.7313	0.6006	<b>6.3</b>
H(24)	0.1133	0.7465	0.5562	<b>6.3</b>
H(25)	0.0128	0.7612	0.6148	<b>9.0</b>
H(26)	-0.0175	0.6892	0.5870	<b>9.0</b>
H(27)	0.0356	0.6780	0.6317	<b>9.0</b>
H(28)	0.2099	0.3167	0.6178	<b>10.7</b>
H(29)	0.1936	0.2961	0.6677	<b>10.7</b>
H(30)	0.0477	0.3412	0.6626	<b>12.4</b>
H(31)	0.0641	0.3608	0.6125	<b>12.4</b>
H(32)	0.0647	0.2748	0.6283	<b>12.4</b>
H(33)	0.2063	0.3945	0.7343	<b>18.9</b>
H(34)	0.2262	0.4829	0.7304	<b>18.9</b>
H(35)	0.0855	0.4624	0.7566	<b>17.2</b>
H(36)	0.0810	0.5036	0.7104	<b>17.2</b>
H(37)	0.0609	0.4151	0.7140	<b>17.2</b>
H(38)	0.3589	0.3523	0.6796	<b>14.4</b>
H(39)	0.3561	0.3643	0.6282	<b>14.4</b>
H(40)	0.4503	0.4005	0.6563	<b>18.0</b>
H(41)	0.3834	0.4609	0.6352	<b>18.0</b>
H(42)	0.3855	0.4494	0.6867	<b>18.0</b>

Supporting dataAnisotropic thermal parameters ( $\text{\AA}^2$ )

The temperature factor is given by:  $T = \exp[-2\pi^2 \sum_i \sum_j U_{ij} h_i h_j a_i^* a_j^*]$

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
Pt	0.0555(2)	0.0527(2)	0.0433(2)	0.0069(3)	-0.0049(2)	-0.0047(3)
P(1)	0.0530(18)	0.0491(17)	0.0496(16)	-0.0057(15)	-0.0012(14)	-0.0013(15)
P(2)	0.115(3)	0.087(3)	0.079(2)	0.038(2)	-0.029(2)	0.011(2)
C(1)	0.060(7)	0.052(7)	0.049(6)	0.001(6)	0.001(6)	-0.007(5)
C(2)	0.044(7)	0.064(8)	0.061(7)	0.007(6)	-0.007(6)	-0.005(6)
C(3)	0.063(8)	0.048(7)	0.048(6)	0.005(6)	-0.010(6)	-0.006(6)
C(4)	0.058(7)	0.082(8)	0.062(7)	0.004(7)	-0.004(7)	-0.026(6)
C(5)	0.070(9)	0.113(12)	0.064(8)	-0.002(8)	-0.022(7)	-0.039(8)
C(6)	0.080(10)	0.094(9)	0.046(6)	0.007(8)	-0.014(7)	-0.026(7)
C(7)	0.049(7)	0.075(8)	0.041(6)	-0.001(6)	0.003(5)	-0.019(6)
C(8)	0.050(7)	0.050(7)	0.046(6)	0.000(6)	-0.009(6)	-0.005(6)
C(9)	0.056(7)	0.057(8)	0.048(7)	-0.007(6)	0.004(6)	-0.007(6)
C(10)	0.073(8)	0.062(8)	0.042(6)	-0.000(7)	-0.000(6)	-0.003(6)
C(11)	0.062(8)	0.067(8)	0.052(7)	-0.011(6)	-0.001(6)	-0.015(6)
C(12)	0.060(7)	0.069(8)	0.052(7)	-0.004(7)	0.005(6)	-0.011(7)
C(13)	0.060(6)	0.060(7)	0.050(5)	0.003(7)	-0.010(7)	-0.006(6)
C(14)	0.082(10)	0.106(11)	0.064(8)	0.022(8)	-0.008(7)	-0.025(7)
C(15)	0.060(9)	0.137(13)	0.088(10)	0.031(9)	-0.015(7)	-0.024(10)
C(16)	0.045(8)	0.129(12)	0.114(11)	0.011(9)	-0.031(8)	-0.040(11)
C(17)	0.080(10)	0.104(12)	0.091(10)	-0.007(9)	-0.032(8)	-0.040(8)

C(18)	0.056(6)	0.068(7)	0.050(6)	0.009(8)	0.002(6)	-0.009(6)
C(19)	0.062(8)	0.064(8)	0.062(8)	-0.014(7)	0.002(7)	-0.015(7)
C(20)	0.061(8)	0.061(8)	0.059(8)	0.003(7)	-0.007(6)	-0.008(6)
C(21)	0.064(8)	0.057(8)	0.063(8)	-0.011(7)	-0.006(7)	-0.002(6)
C(22)	0.060(8)	0.064(8)	0.053(7)	-0.012(7)	0.005(6)	-0.001(6)
C(23)	0.059(8)	0.052(7)	0.035(6)	-0.000(6)	0.003(5)	0.000(5)
C(24)	0.093(9)	0.065(8)	0.051(7)	-0.006(8)	-0.002(7)	-0.006(6)
C(25)	0.146(15)	0.055(8)	0.038(7)	-0.012(9)	0.015(8)	-0.009(6)
C(26)	0.113(11)	0.064(8)	0.053(8)	0.004(9)	0.035(9)	0.002(6)
C(27)	0.078(9)	0.057(7)	0.050(7)	0.016(7)	0.020(6)	0.000(6)
C(28)	0.072(8)	0.050(7)	0.031(5)	-0.012(6)	-0.003(6)	0.003(5)
C(29)	0.050(8)	0.061(8)	0.045(6)	0.002(6)	-0.003(5)	0.011(6)
C(30)	0.060(7)	0.062(8)	0.054(7)	0.010(7)	0.001(7)	0.002(6)
C(31)	0.050(7)	0.061(7)	0.060(7)	-0.012(6)	-0.009(6)	0.002(6)
C(32)	0.095(10)	0.084(10)	0.065(8)	0.002(8)	-0.010(7)	0.009(7)
C(33)	0.083(9)	0.078(9)	0.071(8)	-0.019(8)	0.014(8)	0.014(7)
C(34)	0.056(9)	0.178(16)	0.122(12)	-0.037(9)	0.009(8)	-0.023(12)
C(35)	0.076(9)	0.057(8)	0.064(8)	-0.002(7)	-0.008(7)	-0.007(6)
C(36)	0.095(10)	0.093(10)	0.096(10)	0.026(8)	-0.015(9)	-0.029(8)
C(37)	0.197(17)	0.066(9)	0.077(9)	0.051(13)	0.006(12)	0.010(7)
C(38)	0.172(17)	0.097(12)	0.122(13)	-0.011(14)	0.008(14)	-0.003(10)
C(39)	0.46(4)	0.085(12)	0.051(10)	0.03(2)	-0.064(18)	0.007(9)
C(40)	0.30(3)	0.132(19)	0.114(14)	0.000(20)	0.096(18)	-0.022(12)

Supplementary material

Intermolecular distances ( $\text{\AA}$ ) for non-hydrogen atoms

atom	atom	distance	atom	atom	distance
C6	C18 <sup>i</sup>	3.53(2)	C10	C10 <sup>i</sup>	3.60(2)
C6	C19 <sup>i</sup>	3.53(2)	C20	C27 <sup>iii</sup>	3.52(1)
C7	C32 <sup>ii</sup>	3.60(2)			

Symmetry code:

(i) 1-x, 1-y, 1-z; (ii)  $\frac{1}{2}$ -x, - $\frac{1}{2}$ +y, z; (iii)  $\frac{1}{2}$ +x, y, 1 $\frac{1}{2}$ -z

Supporting data

## Torsion angles (°)

Pt	P1	C31	C32	-178.9(7)	C12	C13	C18	C19	-2(2)
Pt	P1	C33	C34	-60(1)	C13	C14	C15	C16	-1(2)
Pt	P1	C35	C36	-65(1)	C13	C18	C17	C16	-2(2)
Pt	P2	C37	C38	-56(1)	C13	C18	C19	C20	-171(12)
Pt	P2	C39	C40	56(2)	C14	C13	C18	C17	1(2)
Pt	P2	C41	C42	53.7(2)	C14	C13	C18	C19	178(1)
Pt	C1	C2	C3	-38(17)	C14	C15	C16	C17	0(2)
Pt	C30	C29	C28	-27(19)	C15	C14	C13	C18	1(2)
P1	Pt	P2	C37	-28(2)	C15	C16	C17	C18	1(2)
P1	Pt	P2	C39	-153(2)	C16	C17	C18	C19	-179(1)
P1	Pt	P2	C41	74(2)	C17	C18	C19	C20	5(13)
P1	Pt	C1	C2	84(5)	C18	C19	C20	C21	-27(32)
P1	Pt	C30	C29	-113(7)	C19	C20	C21	C22	3(48)
P2	Pt	P1	C31	43(2)	C20	C21	C22	C23	11(49)
P2	Pt	P1	C33	-73(2)	C21	C22	C23	C24	7(22)
P2	Pt	P1	C35	166(2)	C21	C22	C23	C28	-172(21)
P2	Pt	C1	C2	-96(5)	C22	C23	C24	C25	179(1)
P2	Pt	C30	C29	67(7)	C22	C23	C28	C27	-180(1)
C1	Pt	P1	C31	52.4(4)	C22	C23	C28	C29	0(1)
C1	Pt	P1	C33	-63.6(5)	C23	C24	C25	C26	1(2)
C1	Pt	P1	C35	174.8(5)	C23	C28	C27	C26	0(1)
C1	Pt	P2	C37	-36.8(7)	C23	C28	C29	C30	34(14)

C1	Pt	P2	C39	-163(1)	C24	C23	C28	C27	1(1)
C1	Pt	P2	C41	65.2(3)	C24	C23	C28	C29	-180(1)
C1	Pt	C30	C29	-18(8)	C24	C25	C26	C27	0(2)
C1	C2	C3	C4	-122(13)	C25	C24	C23	C28	-1(2)
C1	C2	C3	C8	58(13)	C25	C26	C27	C28	-1(2)
C2	C1	Pt	C30	-11(7)	C26	C27	C28	C29	-180(1)
C2	C3	C4	C5	180(1)	C27	C28	C29	C30	-146(14)
C2	C3	C8	C7	-177(1)	C30	Pt	P1	C31	-137.2(5)
C2	C3	C8	C9	1(2)	C30	Pt	P1	C33	106.9(5)
C3	C4	C5	C6	-1(2)	C30	Pt	P1	C35	-14.7(5)
C3	C8	C7	C6	-4(2)	C30	Pt	P2	C37	152.7(7)
C3	C8	C9	C10	157(12)	C30	Pt	P2	C39	27(1)
C4	C3	C8	C7	3(2)	C30	Pt	P2	C41	-105.2(4)
C4	C3	C8	C9	-179(1)	C31	P1	C33	C34	180(1)
C4	C5	C6	C7	0(2)	C31	P1	C35	C36	60.1(9)
C5	C4	C3	C8	0(2)	C32	C31	P1	C33	-58.5(9)
C5	C6	C7	C8	3(2)	C32	C31	P1	C35	53.0(9)
C6	C7	C8	C9	178(1)	C33	P1	C35	C36	170.7(8)
C7	C8	C9	C10	-25(13)	C34	C33	P1	C35	67(1)
C8	C9	C10	C11	1(36)	C37	P2	C39	C40	-74(2)
C9	C10	C11	C12	119(48)	C37	P2	C41	C42	171.1(4)
C10	C11	C12	C13	-103(48)	C38	C37	P2	C39	76(2)
C11	C12	C13	C14	-2(17)	C38	C37	P2	C41	-172(1)
C11	C12	C13	C18	177(16)	C39	P2	C41	C42	-81.7(8)
C12	C13	C14	C15	-180(1)	C40	C39	P2	C41	-170(2)

Supporting data

Least-squares mean planes (deviations in Å)

<u>Plane 1</u>	Defining atoms	Distance	Other atoms	Distance
	Pt	-0.000(1)		
	P1	-0.00(3)		
	P2	-0.013(4)		
	C1	0.148(10)		
	C30	0.183(11)		

Mean deviation from plane: 0.069 Å;  $\chi^2$ , 497

<u>Plane 2</u>	Defining atoms	Distance	Other atoms	Distance
	C3	-0.008(10)	C2	-0.036
	C4	-0.008(12)	C9	0.040
	C5	0.009(13)		
	C6	0.009(12)		
	C7	-0.019(11)		
	C8	0.018(10)		

Mean deviation from plane: 0.012 Å;  $\chi^2$ , 7.8

<u>Plane 3</u>	Defining atoms	Distance	Other atoms	Distance
	C13	0.001(10)	C12	0.014
	C14	0.007(14)	C19	0.031
	C15	-0.008(15)		
	C16	-0.004(16)		
	C17	0.012(14)		
	C18	-0.007(11)		

Mean deviation from plane: 0.006 Å;  $\chi^2$ , 1.6

<u>Plane 4</u>	Defining atoms	Distance	Other atoms	Distance
	C23	0.005(10)	C22	0.013
	C24	-0.008(11)	C29	0.002
	C25	0.003(12)		
	C26	0.004(11)		
	C27	-0.004(10)		
	C28	-0.000(9)		

Mean deviation from plane: 0.004 Å;  $\chi^2$ , 1.1

<u>Plane</u> 5	Defining atoms	Distance	Other atoms	Distance
	Pt	-0.001(1)	P1	2.182
	C1	-0.062(10)	P2	-2.193
	C2	-0.018(11)	C4	0.183
	C3	0.141(10)	C5	0.343
	C8	0.255(10)	C6	0.484
	C9	0.193(10)	C7	0.468
	C10	0.109(11)	C14	-0.191
	C11	-0.004(11)	C15	-0.270
	C12	-0.071(11)	C16	-0.283
	C13	-0.148(10)	C17	-0.222
	C18	-0.175(11)	C24	0.111
	C19	-0.093(12)	C25	0.164
	C20	-0.012(11)	C26	0.210
	C21	0.053(11)	C27	0.206
	C22	0.092(11)		
	C23	0.126(10)		
	C28	0.168(9)		
	C29	0.173(10)		
	C30	0.122(10)		

Mean deviation from plane: 0.106 Å;  $\chi^2$ , 3828

Dihedral angles between least-squares planes:

plane	plane	angle	plane	plane	angle
2	1	101.3°	4	3	1.4°
3	1	71.7	5	1	74.3
3	2	171.1	5	2	172.3
4	1	72.3	5	3	2.7
4	2	170.7	5	4	2.1