Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2)

$B_{eq} = (8\pi^2/3)\sum\sum U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ (Fischer & Tillmans, 1988).

	x	y	z	B_{eq}
Pd	0	0	0	3.79 (4)
P	0.1356 (2)	0.1083 (2)	0.1887 (3)	3.19 (8)
C(11)	0.1440 (8)	0.1211 (7)	0.4164 (11)	4.9 (4)
C(12)	0.0265 (10)	0.1255 (9)	0.3742 (16)	8.2 (6)
C(13)	0.2116 (10)	0.2081 (8)	0.5403 (14)	8.2 (6)
C(14)	0.1919 (10)	0.0290 (8)	0.5277 (14)	8.4 (6)
C(21)	0.2769 (7)	0.0657 (7)	0.2424 (13)	4.5 (4)
C(22)	0.3797 (7)	0.1141 (8)	0.4027 (14)	6.9 (5)
C(23)	0.2792 (9)	0.0760 (8)	0.0667 (16)	7.7 (6)
C(24)	0.2851 (9)	−0.0433 (8)	0.2780 (18)	7.8 (6)
C(31)	0.1081 (7)	0.2344 (6)	0.0769 (12)	4.6 (4)
C(32)	0.2042 (9)	0.3048 (7)	0.1616 (15)	7.2 (5)
C(33)	0.0650 (9)	0.2196 (8)	−0.1282 (14)	7.6 (6)
C(34)	0.0099 (10)	0.2807 (8)	0.0753 (16)	8.6 (6)

and an angle P—Pd—P of 180.0°. The structures of bulky tertiary phosphine-coordinated Pd or Pt compounds have been determined by several authors to study the steric effects controlling the reactivity of zerovalent noble-metal complexes. The angle P—Pd—P obtained in this study was equal to that found in the same ligands coordinating a Pt compound (Moynihan & Chieh, 1979), and was 3–4° larger than those in the similar Pd or Pt compound with tertiary phosphine ligands consisting of two *tert*-butyl groups and one phenyl group (Otsuka, Yoshida, Matsuda & Nakatsu, 1976; Immirzi & Musco, 1974). The angles in Table 2 show that in each *tert*-butyl group the P—C—C′ angle for the methyl group at the *trans* position to the Pd atom is significantly larger and the angle C—C—C between the other two methyl groups is significantly smaller, reflecting the steric hindrance between the methyl groups.

Table 2. *Bond distances* (Å) *and angles* (°)

Pd—P	2.285 (3)	C(21)—C(22)	1.521 (11)
P—C(11)	1.907 (8)	C(21)—C(23)	1.538 (13)
P—C(21)	1.915 (9)	C(21)—C(24)	1.526 (13)
P—C(31)	1.921 (9)	C(31)—C(32)	1.512 (12)
C(11)—C(12)	1.525 (13)	C(31)—C(33)	1.534 (12)
C(11)—C(13)	1.546 (13)	C(31)—C(34)	1.543 (13)
C(11)—C(14)	1.511 (13)		
P—Pd—P	180.0	P—C(21)—C(22)	117.6 (7)
Pd—P—C(11)	110.1 (3)	P—C(21)—C(23)	108.9 (7)
Pd—P—C(21)	110.8 (3)	P—C(21)—C(24)	107.8 (8)
Pd—P—C(31)	111.8 (3)	C(22)—C(21)—C(23)	108.8 (9)
C(11)—P—C(21)	108.4 (4)	C(22)—C(21)—C(24)	108.6 (9)
C(11)—P—C(31)	108.2 (4)	C(23)—C(21)—C(24)	104.4 (9)
C(21)—P—C(31)	107.4 (4)	P—C(31)—C(32)	117.0 (6)
P—C(11)—C(12)	108.5 (6)	P—C(31)—C(33)	107.4 (7)
P—C(11)—C(13)	116.4 (6)	P—C(31)—C(34)	108.4 (8)
P—C(11)—C(14)	109.0 (7)	C(32)—C(31)—C(33)	109.3 (8)
C(12)—C(11)—C(13)	109.5 (9)	C(32)—C(31)—C(34)	109.4 (8)
C(12)—C(11)—C(14)	104.4 (8)	C(33)—C(31)—C(34)	104.5 (8)
C(13)—C(11)—C(14)	108.4 (8)		

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Dichloro(3-isopropyl-1,2,4,5,5-pentamethylcyclopenta-1,3-diene)platinum(II)

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Abstract. [$PtCl_2(C_{13}H_{22})$], $M_r = 444.29$, monoclinic, $P2_1/c$, $a = 8.599$ (2), $b = 12.070$ (3), $c = 14.583$ (3) Å, $\beta = 94.64$ (2)°, $V = 1508.5$ (6) Å^3, $Z = 4$, $D_x = 1.956$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 101.09$ cm^{-1}, $F(000) = 848$, $T = 296$ K, $R(F) = 3.08\%$ for 2258 observed reflections and 146 parameters. C(5) is 0.493 Å above the plane formed by C(1), C(2), C(3) and C(4). The structure is a square-planar diolefinic complex of Pt^{II}; none of the five elements of the coordination sphere (two Cl ions, Pt and the midpoints of carbon–carbon double bonds) deviate from planarity by more than 0.02 Å.

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Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* ($\text{Å}^2 \times 10^3$)

Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U
Pt	3028.4 (3)	1010.1 (2)	1852.8 (2)	37.7 (1)
Cl(1)	5030 (3)	1940 (2)	1206 (2)	65.2 (8)
Cl(2)	1321 (3)	2467 (2)	1547 (2)	66.3 (8)
C(1)	3914 (10)	−689 (6)	1803 (6)	46 (3)
C(2)	3942 (9)	−292 (6)	2721 (5)	44 (2)
C(3)	2334 (9)	−77 (6)	2908 (5)	42 (2)
C(4)	1402 (8)	−336 (6)	2079 (5)	41 (2)
C(5)	2278 (9)	−1109 (6)	1482 (5)	43 (2)
C(6)	5324 (11)	−991 (8)	1324 (8)	70 (4)
C(7)	5407 (10)	−135 (8)	3351 (6)	60 (3)
C(8)	1734 (10)	284 (7)	3802 (5)	53 (3)
C(9)	1958 (13)	−665 (8)	4488 (7)	68 (4)
C(10)	2360 (13)	1381 (9)	4183 (7)	75 (4)
C(11)	−326 (10)	−191 (8)	1938 (7)	60 (3)
C(12)	1859 (11)	−958 (8)	444 (6)	58 (3)
C(13)	2076 (12)	−2318 (7)	1770 (7)	66 (4)

Experimental. Yellow crystals (0.25 × 0.25 × 0.38 mm) were a gift from Professor Russell P. Hughes at Dartmouth College. Nicolet *R*3*m* diffractometer with graphite monochromator; ω scans; lattice parameters from least-squares fit of 25 reflections ($20 \le 2\theta \le 25°$); empirical absorption correction was applied ($T_{\text{max}}T_{\text{min}} = 2.27$); $2\theta_{\text{max}} = 52°$ ($h = \pm 11$, $k = +15$, $l = +18$); standard reflections 0,10,0, $\bar{6}02$, $\bar{3}29$, variation $< 1\%$. 3293 reflections collected, 2964 unique ($R_{\text{int}} = 1.37\%$), 2258 observed with $F_o > 5.0\sigma(F_o)$, 706 unobserved reflections. Patterson map structure solution; least-squares refinement on F for 146 parameters; all non-H atoms anisotropic, H atoms calculated as idealized contributions [d(C—H) = 0.96 Å, $U(\text{H}) = 1.2U(\text{C})$], $R(F) = 3.08$, $wR(F) = 3.35\%$, $S = 0.962$, $w^{-1} = \sigma(F_o) + gF_o^2$, $g = 0.001$; $(\Delta/\sigma)_{\text{max}} = 0.014$; $\Delta\rho_{\text{max}} = 1.280$, $\Delta\rho_{\text{min}} = -0.643$ e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV); *SHELXTL* computer program (Sheldrick, 1985).

Atomic and equivalent isotropic thermal parameters are given in Table 1 and selected bond lengths and angles are listed in Table 2.* Fig. 1 shows the molecular structure of the compound and Fig. 2 shows the stereo packing diagram.

Related literature. The title compound was an unexpected product (30%) of the room-temperature reaction of 1,2,3-tri-*tert*-butyl-3-vinyl-1-cyclopropene with Zeise's dimer $[\text{Pt}(\text{C}_2\text{H}_4)\text{Cl}_2]_2$ in acetone solution.

Table 2. *Selected bond lengths* (Å) *and angles* (°)

Pt—Cl(1)	2.318 (2)	Pt—Cl(2)	2.310 (2)
Pt—C(1)	2.191 (8)	Pt—C(2)	2.128 (8)
Pt—C(3)	2.143 (7)	Pt—C(4)	2.186 (7)
C(1)—C(2)	1.421 (11)	C(1)—C(5)	1.532 (11)
C(2)—C(3)	1.454 (11)	C(3)—C(4)	1.430 (10)
C(4)—C(5)	1.517 (11)		
Cl(1)—Pt—Cl(2)	92.0 (1)	Cl(1)—Pt—C(1)	99.7 (2)
Cl(1)—Pt—C(2)	110.4 (2)	Cl(1)—Pt—C(3)	147.9 (2)
Cl(1)—Pt—C(4)	157.8 (2)	Cl(2)—Pt—C(1)	157.4 (2)
Cl(2)—Pt—C(2)	151.0 (2)	Cl(2)—Pt—C(3)	113.3 (2)
Cl(2)—Pt—C(4)	101.0 (2)	C(1)—C(2)—C(3)	107.0 (6)
C(2)—C(3)—C(4)	106.2 (6)	C(3)—C(4)—C(5)	110.5 (6)
C(1)—C(5)—C(4)	96.1 (6)		

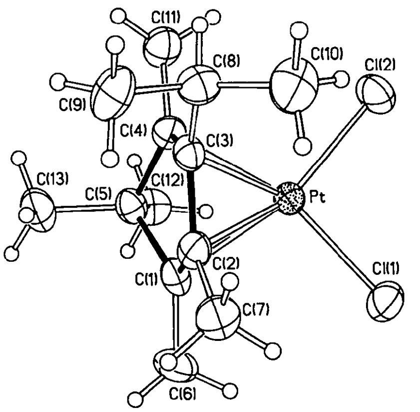

Fig. 1. Molecular structure and labeling scheme for dichloro(3-isopropyl-1,2,3,4,4-pentamethylcyclopenta-1,3-diene)platinum(II).

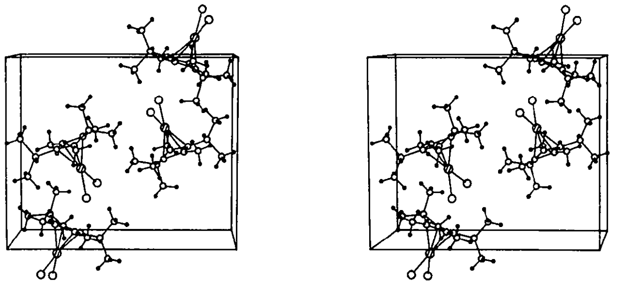

Fig. 2. Stereo packing diagram as viewed down the *a* axis.

The nature of the other products of this reaction and the mechanism of formation of this compound are under continuing investigation (Donovan, Egan, Hughes, Spara, Trujillo & Rheingold, 1990).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and full lists of bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54578 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST0537]

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