is very similar to that of compound II (Tomita, Rosenstein & Jeffrey, 1977).

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trans-Nitrato[2-(di-*tert*-butylphosphino)phenyl]di-*tert*-butylphenylphosphineplatinum(II)

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Abstract. $C_{28}H_{45}NO_3P_2Pt$, orthorhombic, $P2_12_12_1$, a = 8·544 (2), b = 10·589 (3), c = 32·618 (8) Å, Z = 4, D_x = 1·577 g cm^{-3}, V = 2951 (1) Å^3, μ(Mo $K\alpha$) = 49·37 cm^{-1}. The complex has two di-*tert*-butylphenylphosphine ligands, one of which has undergone internal metallation at the *ortho* position of the phenyl group. The resulting highly strained four-membered $PtPC_2$ ring has bond angles of C–Pt–P = 69·7 (5), C–P–Pt = 82·4 (6), C–C–Pt = 106 (1) and C–C–P = 102 (1)°.

Introduction. Measurements were made on a Syntex $P2_1$ diffractometer using monochromatized Mo $K\alpha$ radiation (λ = 0·71069 Å). The cell dimensions and their e.s.d.'s were obtained by least-squares treatment of the setting angles of 15 reflexions with 35° < 2θ < 40°. The structure analysis used the 2263 independent reflexions having 5° < 2θ < 50° and $I > 3\sigma(I)$, where $\sigma(I)$ is the standard deviation derived from counting

Table 1. *Atomic coordinates* (×10^4) *with estimated standard deviations in parentheses*

	x	*y*	*z*
Pt(1)	−1588 (1)	−1233 (1)	−1329 (1)
P(1)	−340 (5)	88 (4)	−866 (1)
P(2)	−2482 (5)	−2924 (4)	−1731 (1)
C(1)	−253 (19)	−1344 (19)	−564 (4)
C(2)	−1054 (19)	−2189 (16)	−809 (6)
C(3)	−1228 (21)	−3426 (14)	−667 (5)
C(4)	−615 (25)	−3773 (22)	−266 (7)
C(5)	178 (29)	−2900 (19)	−36 (7)
C(6)	417 (30)	−1637 (17)	−169 (6)
C(7)	1671 (23)	601 (18)	−1010 (7)
C(8)	2572 (26)	−664 (23)	−1110 (9)
C(9)	1545 (27)	1409 (29)	−1398 (6)
C(10)	2609 (23)	1278 (23)	−699 (6)
C(11)	−1445 (21)	1286 (19)	−567 (5)
C(12)	−732 (31)	1518 (24)	−114 (8)
C(13)	−1471 (32)	2585 (18)	−806 (6)
C(14)	−3122 (25)	778 (26)	−518 (7)
C(15)	−3843 (21)	−2504 (17)	−2187 (6)
C(16)	−2954 (28)	−1758 (18)	−2516 (5)
C(17)	−5126 (20)	−1628 (16)	−1994 (6)
C(18)	−4678 (23)	−3646 (19)	−2357 (6)
C(19)	−3758 (18)	−3963 (16)	−1428 (5)
C(20)	−4707 (19)	−3367 (16)	−1150 (5)
C(21)	−5883 (21)	−4033 (19)	−910 (5)
C(22)	−5999 (25)	−5371 (20)	−995 (7)
C(23)	−5047 (23)	−5893 (15)	−1306 (5)
C(24)	−3947 (20)	−5262 (15)	−1509 (6)
C(25)	−684 (19)	−3821 (20)	−1924 (5)
C(26)	58 (24)	−4568 (20)	−1564 (7)
C(27)	455 (22)	−2819 (20)	−2079 (7)
C(28)	−1066 (24)	−4773 (20)	−2282 (6)
N(1)	−2587 (21)	1130 (16)	−1763 (5)
O(1)	−1694 (17)	102 (11)	−1833 (4)
O(2)	−2166 (26)	2043 (14)	−1973 (6)
O(3)	−3701 (16)	1089 (14)	−1541 (5)

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statistics; a further 760 reflexions were excluded as 'unobserved'. Lorentz, polarization and absorption corrections were applied. The structure was solved with Patterson and electron-density syntheses and refined by least squares. Refinement of coordinates and anisotropic temperature factors for all non-hydrogen atoms converged at $R = 0{\cdot}059$. After transformation of the atomic parameters to those for the enantiomorphous structure, reconvergence gave a final R of 0·043 and R' of 0·054. The function minimized was $\Sigma w(|F_o| - |F_c|)^2$. Modified variances $\sigma^2(I) = \sigma_c^2(I) + (QI)^2$ were used, where σ_c^2 is the variance calculated from counting statistics alone, and weights were calculated from the corresponding expression $w^{-1} = \sigma^2(F) = \sigma_c^2(F) + 0{\cdot}25(QF)^2$. A value of $Q = 0{\cdot}05$ was chosen to give a uniform distribution of $w\Delta^2$ as a function of F_o and $\sin\theta/\lambda$. The final value of $[\Sigma w\Delta^2/(n-m)]^{1/2} = 1{\cdot}42$. Atomic scattering factors were calculated from the analytical approximation and coefficients given in *International Tables for X-ray Crystallography* (1974).

The atomic coordinates and their e.s.d.'s (by inversion of the 9 × 9 block-diagonal least-squares matrix) are given in Table 1.*

Table 2. *Bond lengths* (Å) *and angles* (°) *with their e.s.d.'s*

Pt–P(1)	2·318 (5)	P(1)–Pt–C(2)	69·7 (5)
Pt–P(2)	2·347 (5)	Pt–C(2)–C(1)	106 (1)
Pt–C(2)	2·03 (2)	C(2)–C(1)–P(1)	102 (1)
Pt–O(1)	2·17 (1)	C(1)–P(1)–Pt	82·4 (6)
Pt···O(3)	3·13 (2)	P(1)–Pt–O(1)	96·9 (4)
P(1)–C(1)	1·81 (2)	P(2)–Pt–C(2)	99·2 (5)
P(1)–C(7)	1·86 (2)	P(2)–Pt–O(1)	93·4 (3)
P(1)–C(11)	1·86 (2)	C(1)–C(2)–C(3)	118 (1)
P(2)–C(15)	1·94 (2)	C(2)–C(3)–C(4)	120 (1)
P(2)–C(19)	1·84 (2)	C(3)–C(4)–C(5)	120 (2)
P(2)–C(25)	1·91 (2)	C(4)–C(5)–C(6)	123 (2)
C(1)–C(2)	1·38 (2)	C(5)–C(6)–C(1)	115 (2)
C(2)–C(3)	1·40 (2)	C(6)–C(1)–C(2)	125 (1)
C(3)–C(4)	1·46 (3)	Pt–O(1)–N	115 (1)
C(4)–C(5)	1·37 (3)	O(1)–N–O(2)	112 (2)
C(5)–C(6)	1·42 (3)	O(1)–N–O(3)	122 (1)
C(6)–C(1)	1·44 (3)	O(2)–N–O(3)	126 (2)
N–O(1)	1·35 (2)	Pt–P(1)–C(7)	115·8 (7)
N–O(2)	1·24 (2)	Pt–P(1)–C(11)	121·3 (6)
N–O(3)	1·20 (2)	Pt–P(2)–C(15)	116·7 (6)
C–C(*tert*-butyl)	1·48–1·62 (3)	Pt–P(2)–C(19)	110·5 (5)
C–C(phenyl)	1·33–1·46 (3)	Pt–P(2)–C(25)	107·5 (6)

Discussion. Cheney, Mann, Shaw & Slade (1971) described the preparation of this compound and quoted some molecular dimensions from our earlier unpublished structure determination using film data. The present analysis gives the molecular structure shown in Fig. 1 and the bond lengths and angles with their e.s.d.'s listed in Table 2. The C atom positions have e.s.d.'s of 0·02–0·03 Å.

The main feature of chemical interest is the $PtPC_6$ fused-ring system produced by an internal metallation of one of the di-*tert*-butylphenylphosphine ligands. Similar compounds of iridium have been structurally characterized by Perego, Del Piero, Cesari, Clerici & Perrotti (1973). The large bond-angle deformations which are obviously necessary for four-membered ring formation are evident; C–Pt–P is reduced from its normal value of 90 to 69·7 (5)°, C–P–Pt from its tetrahedral value to 82·4 (6)°, and C–C–Pt and C–C–P angles from 120 to 106 (1) and 102 (1)° respectively. The Pt–P(1) bond seems to suffer a compression as a result of ring strain, its length of 2·318 (5) Å being substantially less than the 2·347 (5) Å length of the bond to the unmetallated phosphine. The C atoms of the metallated phenyl ring do not depart significantly from coplanarity, but the Pt and P(1) atoms show displacements of +0·071 and −0·043 Å from the mean plane of the six C atoms.

The nitrate ligand seems to be bonded in a normal unidentate fashion (Addison, Logan, Wallwork & Garner, 1971), with Pt–O(1) = 2·17 (1) Å, and the Pt···O(3) contact of 3·13 (2) Å essentially non-bonding.

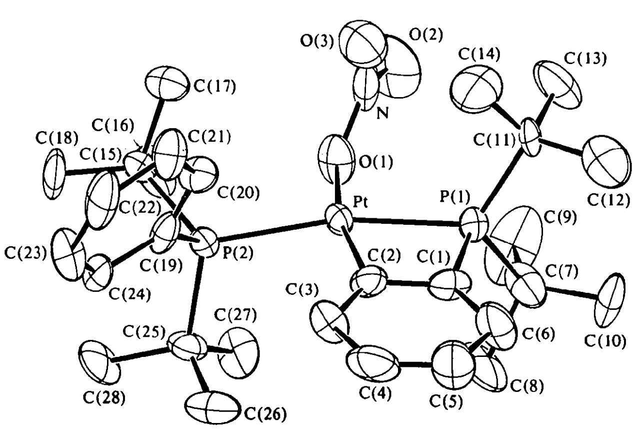

Fig. 1. *ORTEP* drawing of the molecule with atom numbering.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32846 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.