

Table 1. Fractional coordinates and vibration parameters ($\text{\AA}^2 \times 10^3$) with their e.s.d.'s

The temperature factors are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{23}klb^*c^* + 2U_{31}lhc^*a^* + 2U_{12}hka^*b^*)] \text{ or } \exp[-2\pi^2U_{\text{iso}}(2\sin\theta/\lambda)^2]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
Pt	0	0	0	32 (1)	34 (1)	19 (5)	3 (1)	0 (1)	7 (1)
P	0.2294 (9)	0.1764 (6)	0.1850 (9)	45 (3)	50 (3)	39 (6)	4 (3)	0 (2)	14 (3)

	x	y	z	U_{iso}		x	y	z	U_{iso}
O	-0.071 (3)	0.111 (2)	-0.152 (3)	62 (5)	C(8)	0.011 (4)	0.204 (3)	0.349 (4)	63 (7)
C(1)	0.179 (4)	0.285 (3)	0.052 (4)	57 (7)	C(9)	0.224 (7)	0.113 (5)	0.517 (8)	118 (15)
C(2)	0.020 (3)	0.232 (2)	-0.101 (3)	46 (6)	C(10)	0.319 (6)	0.344 (4)	0.521 (6)	91 (11)
C(3)	-0.039 (4)	0.300 (3)	-0.214 (4)	64 (7)	C(11)	0.464 (4)	0.191 (3)	0.215 (4)	58 (7)
C(4)	0.057 (5)	0.423 (3)	-0.174 (5)	77 (9)	C(12)	0.451 (5)	0.168 (3)	0.019 (5)	73 (8)
C(5)	0.221 (5)	0.483 (4)	-0.013 (6)	86 (10)	C(13)	0.497 (5)	0.088 (3)	0.305 (6)	83 (10)
C(6)	0.275 (5)	0.409 (3)	0.095 (5)	75 (9)	C(14)	0.612 (5)	0.311 (3)	0.325 (5)	77 (9)
C(7)	0.200 (3)	0.208 (2)	0.399 (3)	46 (6)					

Table 2. Bond lengths and angles with their e.s.d.'s

Pt-P	2.300 (5) \AA	P-Pt-O	83.2 (5)°
Pt-O	1.97 (2)	Pt-P-C(3)	100.1 (8)
P-C(1)	1.80 (3)	P-C(1)-C(2)	113 (2)
C(1)-C(2)	1.38 (3)	C(1)-C(2)-O	122 (2)
C(2)-O	1.35 (3)	C(2)-O-Pt	122 (1)
P-C(7)	1.85 (3)	Pt-P-C(7)	109.4 (7)
P-C(11)	1.89 (3)	Pt-P-C(11)	116.3 (9)

C-C (*tert*-butyl) 1.51-1.61 (4) \AA

C-C (benzene ring) 1.34-1.45 (4)

shown in Fig. 1 and the more important bond lengths and angles are given in Table 2. The molecule occupies a crystallographic centre of symmetry with all atoms,

except those of the *tert*-butyl substituents, coplanar to within 2σ . However, the geminal *tert*-butyl groups are only approximately related by a mirror through the molecular plane, and the molecule departs significantly from C_{2h} symmetry.

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References

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Chloro[2-(diphenylphosphinato)phoxymethyl]pyridineplatinum(II)

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Abstract. $\{\text{Pt}[\text{CH}_2\text{OC}_6\text{H}_4\text{PPH}_2](\text{C}_6\text{H}_5\text{N})\text{Cl}\}$, $\text{C}_{25}\text{H}_{21}\text{ClN}\text{OPt}$, monoclinic, $P2_1/a$; $a = 18.62$ (2), $b = 10.72$ (1), $c = 11.29$ (1) \AA, $\beta = 107.6$ (2)°; $Z = 4$, $D_x = 1.90$ g cm $^{-3}$, $V = 2148$ \AA 3 . The compound contains a six-membered Pt-P-C-C-O-C chelate ring formed by internal metallation of the methyl C atom of a 2-methoxyphenylphosphine ligand. The chelate ring is highly non-planar, with a dihedral angle of 44° between the metal's coordination plane and the $\text{PC}_6\text{H}_4\text{O}$ plane of the metallated ligand. Square-planar coordination is completed by the chloro and pyridine ligands.

Introduction. Cell dimensions were determined from zero-level precession photographs [$\lambda(\text{Mo } K\alpha) = 0.7107$ \AA] and intensities were recorded on Weissenberg photographs of reciprocal-lattice layers $h0l-h7l$. Visual estimation gave 2560 independent F_o which were not corrected for absorption. Solution of the structure by the heavy-atom method and refinement by block-diagonal least squares gave a final R of 10.1%. Atomic coordinates, anisotropic temperature factors for Pt, P and Cl, and isotropic temperature factors for C, N and O were refined with the weighting scheme $w = \frac{1}{15} +$

Table 1. Fractional coordinates and vibration parameters ($\text{\AA}^2 \times 10^3$) with their e.s.d.'s

The temperature factors are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{23}klb^*c^* + 2U_{31}lhc^*a^* + 2U_{12}hka^*b^*)]$ or $\exp[-2\pi^2U_{\text{iso}}(2 \sin \theta/\lambda)^2]$.

	<i>x</i>	<i>y</i>	<i>z</i>	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
Pt	0.16014 (3)	0.00554 (6)	0.11534 (5)	35.9 (3)	43.0 (7)	43.1 (3)	-6.7 (3)	5.1 (3)	1.1 (3)
P	0.20029 (17)	0.13334 (38)	0.26829 (29)	33 (3)	38 (3)	41 (2)	0 (2)	4 (2)	-1 (2)
Cl	0.11426 (26)	-0.15131 (49)	-0.03112 (43)	71 (3)	79 (4)	73 (3)	-33 (3)	4 (2)	0 (2)

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}		<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}
O	0.1368 (7)	-0.1212 (13)	0.3275 (11)	71 (3)	N	0.1284 (6)	0.1329 (12)	-0.0305 (10)	44 (3)
C(1)	0.1619 (7)	0.0933 (15)	0.3900 (12)	43 (3)	C(13)	0.2202 (10)	0.3897 (19)	0.2488 (16)	65 (4)
C(2)	0.1355 (9)	-0.0255 (17)	0.4034 (14)	53 (4)	C(14)	0.3013 (7)	0.1370 (14)	0.3396 (12)	42 (3)
C(3)	0.1017 (10)	-0.0469 (20)	0.4968 (16)	65 (5)	C(15)	0.3480 (8)	0.1687 (16)	0.2696 (14)	52 (4)
C(4)	0.1008 (11)	0.0409 (22)	0.5804 (17)	71 (5)	C(16)	0.4251 (10)	0.1734 (17)	0.3217 (17)	60 (4)
C(5)	0.1269 (10)	0.1566 (18)	0.5710 (16)	63 (5)	C(17)	0.4571 (11)	0.1371 (20)	0.4403 (17)	73 (5)
C(6)	0.1588 (10)	0.1884 (18)	0.4783 (16)	60 (5)	C(18)	0.4108 (9)	0.0995 (18)	0.5120 (15)	62 (4)
C(7)	0.1914 (10)	-0.1137 (19)	0.2586 (16)	68 (5)	C(19)	0.3338 (9)	0.1013 (18)	0.4600 (14)	58 (4)
C(8)	0.1708 (8)	0.2918 (14)	0.2333 (12)	44 (4)	C(20)	0.0554 (9)	0.1462 (17)	-0.0988 (15)	60 (4)
C(9)	0.0936 (8)	0.3138 (15)	0.1786 (13)	45 (4)	C(21)	0.0305 (9)	0.2419 (18)	-0.1834 (15)	59 (4)
C(10)	0.0660 (9)	0.4326 (18)	0.1406 (14)	60 (4)	C(22)	0.0794 (9)	0.3370 (17)	-0.1919 (15)	55 (4)
C(11)	0.1186 (11)	0.5301 (20)	0.1561 (18)	70 (5)	C(23)	0.1540 (10)	0.3266 (17)	-0.1209 (15)	57 (4)
C(12)	0.1933 (14)	0.5059 (17)	0.2012 (23)	79 (6)	C(24)	0.1774 (9)	0.2286 (16)	-0.0425 (14)	51 (4)

Table 2. Bond lengths and angles with their e.s.d.'s

Pt—P	2.153 (4) Å	P—Pt—C(7)	79.2 (6)°
Pt—C(7)	2.00 (2)	P—Pt—N	99.4 (4)
Pt—N	2.08 (1)	C(7)—Pt—Cl	93.8 (6)
Pt—Cl	2.332 (5)	N—Pt—Cl	87.5 (4)
P—C(1)	1.78 (2)	Pt—P—C(1)	110.0 (5)
P—C(8)	1.79 (2)	Pt—P—C(8)	114.7 (4)
P—C(14)	1.81 (2)	Pt—P—C(14)	115.7 (5)
C(2)—O	1.34 (3)	C(2)—O—C(7)	117 (2)
O—C(7)	1.46 (3)	O—C(7)—Pt	113 (1)
N—C(20)	1.35 (2)		
N—C(24)	1.41 (3)		

C—C (benzene or pyridine ring) 1.32–1.44 (3) Å

0.0002 F_o^3 . Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). The final atomic coordinates and vibration parameters with their e.s.d.'s are given in Table 1.*

Discussion. Jones, Shaw & Turtle (1974) have shown that complexes of platinum(II) with 2-methoxyphenylphosphines undergo internal metallation of the methoxy substituent. According to the reaction conditions, there may be either metallation of the methyl C atom or demethylation and metallation of the O atom. This paper describes the structure analysis of a C-metallated compound and the preceding paper describes that of an O-metallated compound.

The molecular structure and atom numbering are shown in Fig. 1 and the more important bond lengths and angles are listed in Table 2. The six-membered chelate ring is highly non-planar, the mean coordination plane of the metal and the mean plane of the *ortho*-

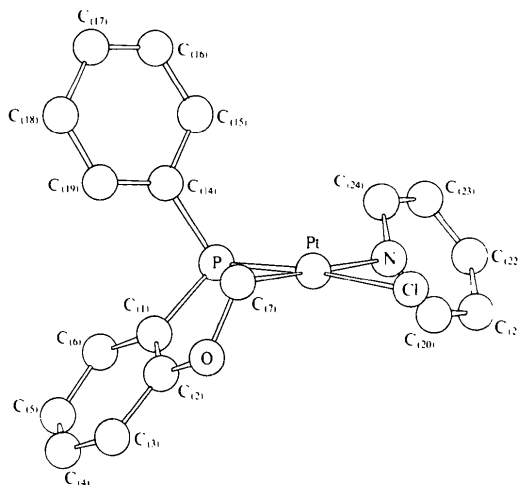


Fig. 1. The molecular structure and atom numbering. For clarity the second phenyl substituent attached to phosphorus has been omitted. Its atom numbers are C(8) to C(13).

$\text{PC}_6\text{H}_4\text{O}$ system of the metallated ligand making a dihedral angle of 44° . The O atom lies 1.27 \AA out of the coordination plane of Pt and C(7) is 0.52 \AA from the $\text{PC}_6\text{H}_4\text{O}$ plane. The mean plane of the pyridine ligand has a dihedral angle of 56° with the coordination plane of platinum.

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References

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31975 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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