

Cl—Pt—Cl (shown in Fig. 2) is consistent with this model. The sulfoxide O—Pt distance in this complex is 3.115 (6) Å. The Pt—S—O angle is 116.1 (3)°.

The generous provision of computer time by the University of Illinois at Chicago Circle Computer Center is gratefully acknowledged.

References

- CHRISTENSEN, B. W. & KJAER, A. (1965). *Chem. Commun.* pp. 225–226.
- CHURCHILL, M. R. (1973). *Inorg. Chem.* **12**, 1213–1214.
- CHURCHILL, M. R. & DEBOER, B. G. (1973). *Inorg. Chem.* **12**, 525–531.
- CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.
- CROMER, D. T. & WABER, J. T. (1965). *Acta Cryst.* **18**, 104–108.
- ENEMARK, J. H. & FELTHAM, R. D. (1974). *Coord. Chem. Rev.* **13**, 339–406.
- FREEMAN, H. C. & GOLOMB, M. W. (1970). *Chem. Commun.* pp. 1523–1524.
- HOFFMANN, R., CHEN, M. M. L., ELIAN, M., ROSSI, A. R. & MINGOS, D. N. P. (1974). *Inorg. Chem.* **13**, 2666–2674.
- RYAN, R. R. & ELLER, P. G. (1976). *Inorg. Chem.* **15**, 494–496.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
- WARREN, R. C., MCCONNELL, J. R. & STEPHENSON, N. C. (1970). *Acta Cryst.* **B26**, 1402–1407.

Acta Cryst. (1977). **B33**, 194–195

trans-Bis[2-(di-*tert*-butylphosphinato)phenoxy]platinum(II)

BY K. H. P. O'FLYNN AND W. S. McDONALD

Department of Inorganic and Structural Chemistry, The University, Leeds LS2 9JT, England

(Received 14 April 1976; accepted 27 June 1976)

Abstract. {Pt[OC₆H₄P(C₄H₉)₂]₂}, C₂₈H₄₄O₂P₂Pt, triclinic, *P* $\bar{1}$; *a* = 8.60 (1), *b* = 11.93 (1), *c* = 8.03 (1) Å, α = 94.3 (1), β = 110.5 (1), γ = 109.1 (1)°; *Z* = 1, *D_x* = 1.56 g cm⁻³, *V* = 712.3 Å³. The centrosymmetric molecules contain two Pt—P—C—C—O chelate rings resulting from internal *O*-metallation and demethylation of 2-methoxyphenylphosphine ligands. Except for the *tert*-butyl substituents, all atoms of a molecule are coplanar to within the accuracy of the analysis.

Introduction. Cell dimensions were determined from zero-level precession and Weissenberg photographs [$\lambda(\text{Mo } K\alpha) = 0.7107 \text{ \AA}$] and intensities were recorded on Weissenberg photographs of reciprocal-lattice levels *hk0*–*hk8*. Visual estimation gave 2164 independent *F_o*, which were not corrected for absorption. Solution of the structure was by the heavy-atom method and full-matrix least-squares refinement gave a final *R* of 12.0%. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974), and atomic coordinates, anisotropic temperature factors for Pt and P, and isotropic temperature factors for C and O were refined. The final atomic parameters with their e.s.d.'s are listed in Table 1.*

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31973 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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 of an *O*-metallated compound and the following paper that of a *C*-metallated compound.

The molecular structure and atom numbering are

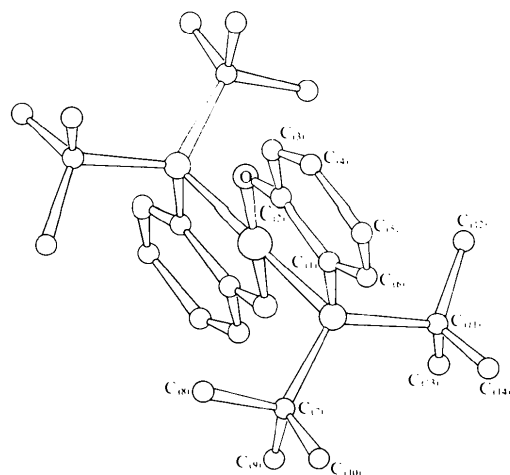


Fig. 1. The molecular structure and atom numbering.

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.

We are grateful to the Science Research Council for financial support.

References

- International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
 JONES, C. E., SHAW, B. L. & TURTLE, B. L. (1974). *J. Chem. Soc. Dalton*, pp. 992-999.

Acta Cryst. (1977). B33, 195-196

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

BY K. H. P. O'FLYNN AND W. S. McDONALD

Department of Inorganic and Structural Chemistry, The University, Leeds LS2 9JT, England

(Received 14 April 1976; accepted 27 June 1976)

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 $w = \frac{1}{15} +$