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Dichloro{*N*-(diphenylphosphino)-*N*-[(diphenylphosphoryl)methyl]pyridin-2-amine-κ^2N,N'}-platinum(II)

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The title compound, $[PtCl_2(C_{30}H_{26}N_2OP_2)]$, is a mononuclear Pt^{II} complex. The Pt atom is coordinated by one pyridine N atom, one P atom and two Cl atoms, which form a distorted square plane around the Pt^{II} atom.

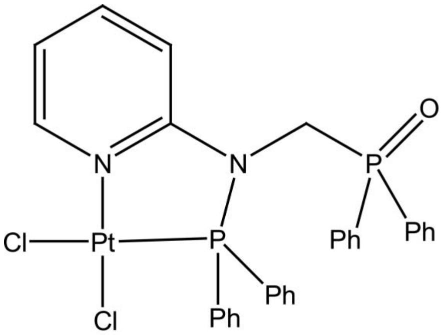
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.012 Å
R factor = 0.025
wR factor = 0.051
Data-to-parameter ratio = 12.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In the last decade, phosphine ligands have been used to synthesize mono- and binuclear complexes (Zhang & Cheng, 1996). Recently, their metallic complexes have also been used as catalytic precursors (Volkis *et al.*, 2005). Much attention has also been paid to multidentate ligands (Christensen *et al.*, 1974; Fryzuk & MacNeil, 1981). We report here an unexpected Pt^{II} complex, (I).



(I)

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Atoms P1, N1, Cl1 and Cl2 deviate from the least-squares plane defined by these atoms by −0.0532 (5), 0.0537 (4), −0.0464 (6) and 0.0459 (5) Å, respectively. These atoms form a distorted square plane around the Pt1 atom. Atom Pt1 is at a distance of 0.0344 (5) Å from this plane. It is interesting that the P═N bond has been oxidized to P═O.

Experimental

Chlorodiphenylphosphine (11 g, 50 mmol) in toluene was added to a toluene solution of *N*,*N*-di-2-pyridylmethylenediamine (5 g, 25 mmol) in an ice bath. The mixture was stirred overnight and then condensed to obtain the phosphine ligand. The title complex, (I), was obtained from the treatment of that ligand (142 mg, 0.25 mmol) with $Pt(COD)Cl_2$ (where COD is 1,5-cyclooctadiene) (94 mg, 0.25 mmol) in dichloromethane (yield 135 mg, 71%; m.p. 413–415 K). Single crystals of (I) were obtained by slow evaporation of a dichloromethane solution.

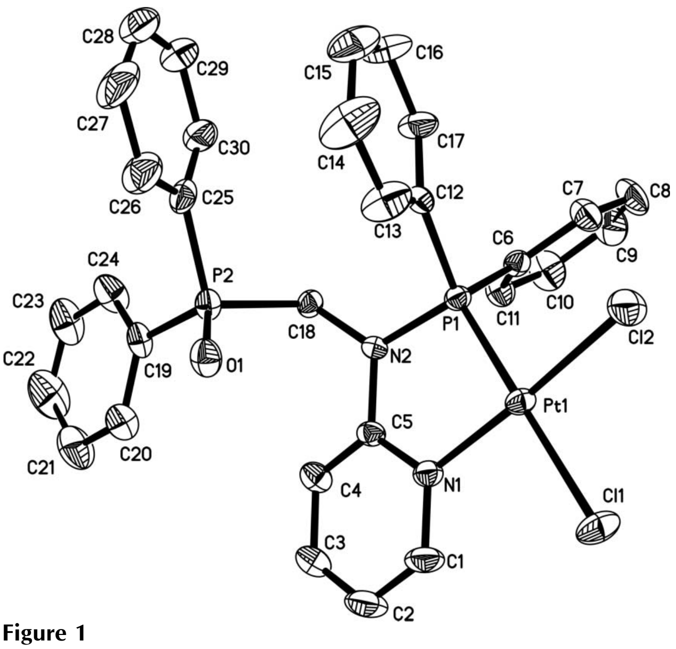


Figure 1

The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

Crystal data

$[PtCl_2(C_{30}H_{26}N_2OP_2)]$
$M_r = 758.46$
Monoclinic, $P2_1$
$a = 8.3946\ (9)$ Å
$b = 11.4865\ (12)$ Å
$c = 15.0673\ (17)$ Å
$\beta = 91.789\ (2)^\circ$
$V = 1452.1\ (3)$ Å^3
$Z = 2$
$D_x = 1.735$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 5.15$ mm^{-1}
$T = 294\ (2)$ K
Plate, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.332$, $T_{max} = 0.600$
8226 measured reflections
4221 independent reflections
3839 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.4^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.051$
$S = 0.91$
4221 reflections
344 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2)]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}
Absolute structure: Flack (1983), with 1107 Friedel pairs
Flack parameter: 0.000 (6)

Table 1

Selected geometric parameters (Å, °).

Pt1—N1	2.030 (5)	P1—C6	1.813 (5)
Pt1—P1	2.1775 (13)	P2—O1	1.485 (4)
Pt1—Cl2	2.2912 (17)	P2—C25	1.798 (7)
Pt1—Cl1	2.3691 (14)	P2—C19	1.806 (6)
P1—N2	1.687 (5)	P2—C18	1.864 (5)
P1—C12	1.812 (6)		
N1—Pt1—P1	83.85 (13)	N2—P1—Pt1	101.78 (16)
N1—Pt1—Cl2	176.78 (14)	C12—P1—Pt1	120.5 (2)
P1—Pt1—Cl2	93.08 (6)	C6—P1—Pt1	114.21 (18)
N1—Pt1—Cl1	94.44 (14)	O1—P2—C25	112.4 (3)
P1—Pt1—Cl1	175.40 (7)	O1—P2—C19	112.9 (3)
Cl2—Pt1—Cl1	88.70 (7)	C25—P2—C19	107.4 (3)
N2—P1—C12	108.1 (4)	O1—P2—C18	112.5 (2)
N2—P1—C6	106.6 (2)	C25—P2—C18	105.5 (3)
C12—P1—C6	104.7 (4)	C19—P2—C18	105.7 (3)

H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methyl H, respectively, and were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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