Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

cis-Dichlorobis(triphenylphosphine-κP)platinum(II)

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Received 2 May 2006
Accepted 4 May 2006

The geometry of the Pt atom in the title compound, $[PtCl_2(C_{18}H_{15}P)_2]$, is square planar. There are two crystallographically independent molecules, *A* and *B*, in the asymmetric unit. The average Pt—P bond distances are 2.2614 (9) (in *A*) and 2.2659 (10) Å (in *B*), with Pt—Cl distances of 2.3463 (8) (in *A*) and 2.3496 (10) Å (in *B*). The molecular structure is stabilized by intermolecular C—H···Cl hydrogen bonds and C—H···π interactions.

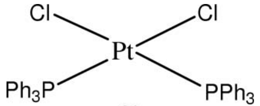
Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.007 Å
R factor = 0.031
wR factor = 0.071
Data-to-parameter ratio = 24.4

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

Comment

cis-Dichlorobis(triphenylphosphine)platinum(II), (I), is an intermediate synthetic material used in the synthesis of other platinum complexes. A number of analogous dichlorobis(triphenylphosphine)platinum(II) complexes have been crystallographically characterized in the past decades, including the structure of the title compound as an acetone solvate (Anderson *et al.*, 1982) and the alternative *trans* isomer (Johansson & Otto, 2000). We report here the unsolvated structure (I) (Figs. 1 and 2, and Table 1).



(I)

The asymmetric unit of (I) contains two crystallographically independent molecules, *A* and *B*, which have similar bond lengths and angles (Figs. 1 and 2). The bond lengths in (I) show normal values (Allen *et al.*, 1987) and agree with the corresponding values found in *cis*-dichlorobis(triphenylphosphine)-platinum(II) acetone solvate (Anderson *et al.*, 1982). The Pt atom has a square planar coordination in both molecules, the mean deviation from the Pt1—P1—P2—Cl1—Cl2 plane being 0.0579 (1) Å for molecule *A* and 0.139 (1) Å for *B*. Atom Pt1*A* deviates by 0.0002 (1) Å from the mean plane and Pt1*B* by 0.0012 (1) Å.

The average Pt—P bond length [2.2614 (9) Å in *A* and 2.2659 (10) Å in *B*] is a normal single bond and shorter than that found in *trans*-$[PtCl_2(PPh_3)_2]$ [2.316 (11) Å; Johansson & Otto, 2000], whereas the average Pt—Cl bond length [2.3463 (8) Å in *A* and 2.3496 (10) Å in *B*] is longer than that of *trans*-$[PtCl_2(PPh_3)_2]$ [2.2997 (11) Å; Johansson & Otto, 2000]. In addition, the average adjacent bond angle of P—Pt—Cl [88.59 (3)° in *A* and 86.8 (4)° in *B*] is less than that of *trans*-$[PtCl_2(PPh_3)_2]$ (90°; Johansson & Otto, 2000). These geometrical differences can be partly attributed to steric repulsion within the *cis* isomer which is different from that of the *trans* isomer.

doi:10.1107/S1600536806016540

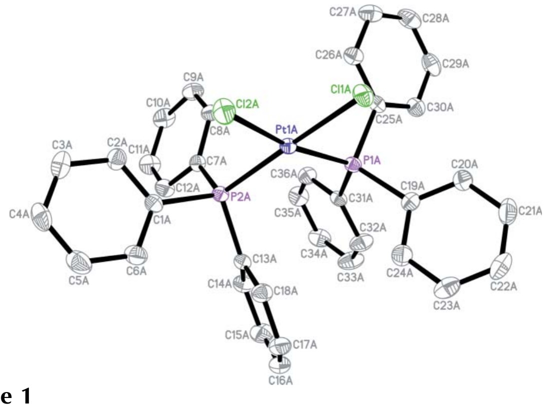


Figure 1
One of the two independent molecules in the asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atomic numbering; H atoms have been omitted for clarity.

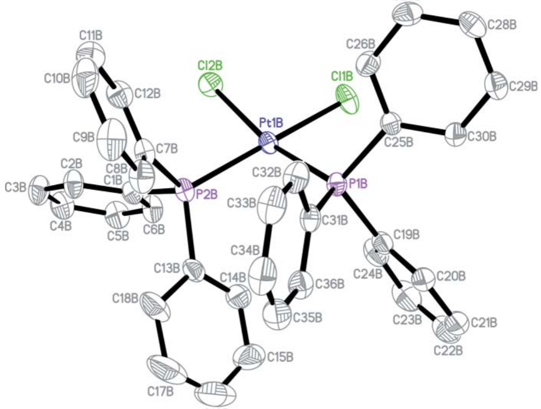


Figure 2
The other independent molecule, showing 30% probability displacement ellipsoids and the atomic numbering; H atoms have been omitted for clarity.

The crystal structure of (I) is stabilized by intermolecular C—H···Cl hydrogen bonds (Table 2 and Fig. 3) which link the molecules into a three-dimensional molecular network. In addition, the packing is stabilized by C—H···π interactions (Table 2).

Experimental

Liriodenine (0.022 g, 0.08 mmol) in methanol (10 ml) was added dropwise to a solution of $Pt(PPh_3)_2Cl_2$ (0.063 g, 0.08 mmol) in methanol (5 ml) and CH_3Cl (5 ml). Refluxing for 6 h with stirring gave a transparent brown–yellow solution. After cooling to room temperature, the solution was filtered and purple plate-shaped single crystals of (I) were obtained after several days at ambient temperature.

Crystal data

$[PtCl_2(C_{18}H_{15}P)_2]$
$M_r = 790.52$
Monoclinic, $P2_1/c$
$a = 32.5958$ (4) Å
$b = 9.6895$ (1) Å
$c = 19.6170$ (2) Å
$\beta = 94.476$ (1)°
$V = 6176.88$ (12) Å^3
$Z = 8$
$D_x = 1.700$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.85$ mm^{-1}
$T = 297$ (2) K
Plate, purple
0.30 × 0.29 × 0.06 mm

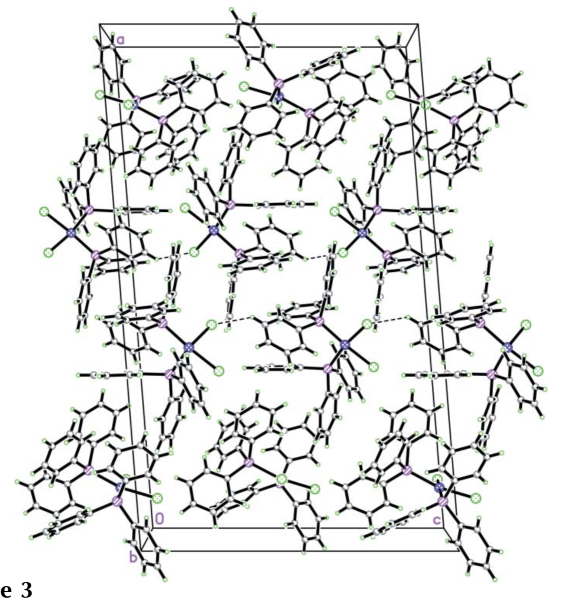


Figure 3
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.255$, $T_{max} = 0.748$
150461 measured reflections
18034 independent reflections
12898 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 30.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.071$
$S = 1.02$
18034 reflections
739 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0197P)^2 + 12.2287P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 1.11$ e Å^{-3}
$\Delta\rho_{min} = -1.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1*A*—P2*A*	2.2515 (8)	P1*A*—C31*A*	1.835 (3)
Pt1*A*—P1*A*	2.2713 (9)	P2*A*—C7*A*	1.817 (3)
Pt1*A*—Cl2*A*	2.3294 (9)	P2*A*—C13*A*	1.817 (3)
Pt1*A*—Cl1*A*	2.3632 (8)	P2*A*—C1*A*	1.838 (4)
Pt1*B*—P2*B*	2.2605 (10)	P1*B*—C19*B*	1.816 (4)
Pt1*B*—P1*B*	2.2713 (10)	P1*B*—C25*B*	1.838 (4)
Pt1*B*—Cl2*B*	2.3483 (10)	P1*B*—C31*B*	1.840 (4)
Pt1*B*—Cl1*B*	2.3509 (11)	P2*B*—C13*B*	1.822 (4)
P1*A*—C25*A*	1.831 (4)	P2*B*—C7*B*	1.825 (4)
P1*A*—C19*A*	1.832 (4)	P2*B*—C1*B*	1.827 (4)
P2*A*—Pt1*A*—P1*A*	99.12 (3)	P1*B*—Pt1*B*—Cl1*B*	86.25 (4)
P2*A*—Pt1*A*—Cl2*A*	89.82 (3)	Cl2*B*—Pt1*B*—Cl1*B*	87.73 (4)
P1*A*—Pt1*A*—Cl2*A*	170.41 (3)	C25*A*—P1*A*—C19*A*	108.55 (17)
P2*A*—Pt1*A*—Cl1*A*	175.57 (3)	C25*A*—P1*A*—C31*A*	98.78 (15)
P1*A*—Pt1*A*—Cl1*A*	83.73 (3)	C19*A*—P1*A*—C31*A*	103.97 (16)
Cl2*A*—Pt1*A*—Cl1*A*	87.56 (3)	C25*A*—P1*A*—Pt1*A*	110.36 (12)
P2*B*—Pt1*B*—P1*B*	99.93 (4)	C7*A*—P2*A*—C13*A*	111.55 (16)
P2*B*—Pt1*B*—Cl2*B*	87.35 (4)	C7*A*—P2*A*—C1*A*	99.94 (16)
P1*B*—Pt1*B*—Cl2*B*	167.58 (4)	C13*A*—P2*A*—C1*A*	103.55 (16)
P2*B*—Pt1*B*—Cl1*B*	171.13 (4)	C13*A*—P2*A*—Pt1*A*	110.06 (11)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C31*B*–C36*B* and C13*B*–C18*B* phenyl rings.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11*A*—H11*A*···Cl2*A*^{i}	0.93	2.75	3.486 (4)	136
C8*B*—H8*BA*···*Cg*1	0.93	2.75	3.395 (6)	127
C36*B*—H36*B*···*Cg*2	0.93	2.75	3.185 (6)	110

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

H atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The highest peak is located 0.97 Å from atom Pt1*B* and the deepest hole 0.55 Å from the same atom.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PLATON* (Spek, 2003) and *PARST* (Nardelli, 1995).

The Natural Science Foundation of Guangxi Province (No. 0429001) and the National Natural Science Foundation of China (Nos. 20361002 and 30460153) are thanked for support. The authors also thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118.

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