Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Chlorotris(triphenylphosphine)platinum(II) perchlorate dichloromethane disolvate

Ning Zhang,[a] Si-Lin Wu,[a] Qian-Yong Cao[a]* and Jing-Hua Liu[b]

[a]Department of Chemistry, Nanchang University, Nanchang 330047, People's Republic of China, and [b]School of Science, Nanchang University, Nanchang 330047, People's Republic of China

Correspondence e-mail: cqyong@ncu.edu.cn

Key indicators

Single-crystal X-ray study
T = 303 K
Mean σ(C–C) = 0.018 Å
Disorder in solvent or counterion
R factor = 0.065
wR factor = 0.180
Data-to-parameter ratio = 17.1

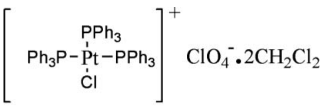
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 December 2005
Accepted 17 January 2006

In the structure of the title complex, $[\mathrm{PtCl(C_{18}H_{15}P)_3}]\mathrm{ClO_4}\cdot 2\mathrm{CH_2Cl_2}$, the coordination polyhedron with platinum as the central atom has a distorted square-planar geometry formed by three P atoms from three triphenylphosphine ligands and one Cl atom.

Comment

Tertiary phosphines such as triphenylphosphine play an important role as ligands in coordination chemistry and are well known to stabilize transition metals in low oxidation states (Vogler & Kunkely, 2002). Platinum(II) complexes incorporating the triphenylphosphine ligand have been well studied (Abram *et al.*, 1999). We have prepared the title compound, (I), and report its structure here.



$$\left[\begin{array}{c}\mathrm{PPh_3}\\ \mathrm{Ph_3P-Pt-PPh_3}\\ \mathrm{Cl}\end{array}\right]^+ \mathrm{ClO_4^-}\cdot 2\mathrm{CH_2Cl_2}$$

(I)

The molecular structure of (I) is shown in Fig. 1. The platinum(II) center adopts distorted square planar geometry; selected bond lengths and angles are given in Table 1. The Pt—P distances are within the normal range (Johansson & Otto, 2000).

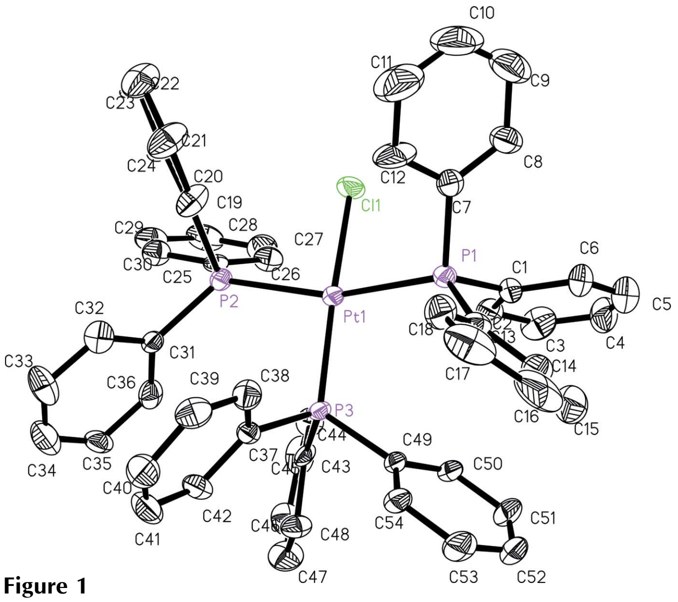


Figure 1
Perspective view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level, and all H atoms, perchlorate anions and solvent dichloromethane molecules have been omitted for clarity.

Experimental

A mixture of $PtCl_2$ (80 mg, 0.3 mmol) and PPh_3 (236 mg, 0.9 mmol) in CH_3CN (30 ml) was heated to reflux for 3 h under a nitrogen atmosphere. The colorless solution was cooled to room temperature, and excess $LiClO_4$ (200 mg, 1.9 mmol) was added and reacted for a further 5 h. The resulting solution was concentrated to 5 ml. Addition of diethyl ether afforded a white solid, which was filtered and washed with water (3 × 20 ml) and diethyl ether (2 × 20 ml). Recrystallization by vapor diffusion of diethyl ether into a dichloromethane solution afforded colorless crystals suitable for X-ray diffraction analysis.

Crystal data

$[PtCl(C_{18}H_{15}P)_3](ClO_4)\cdot 2CH_2Cl_2$
$M_r = 1201.73$
Monoclinic, $P2_1/c$
$a = 17.889\ (5)$ Å
$b = 12.323\ (3)$ Å
$c = 26.217\ (9)$ Å
$\beta = 104.848\ (12)^\circ$
$V = 5586\ (3)$ Å^3
$Z = 4$
$D_x = 1.429$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 992 reflections
$\theta = 2.9$–24.7°
$\mu = 2.83$ mm^{-1}
$T = 303\ (2)$ K
Block, colorless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.493$, $T_{max} = 0.753$
28838 measured reflections
11417 independent reflections
7366 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 26.5^\circ$
$h = -22 \rightarrow 20$
$k = -15 \rightarrow 15$
$l = -32 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.180$
$S = 1.09$
11417 reflections
669 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0887P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 1.46$ e Å^{-3}
$\Delta\rho_{min} = -1.03$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—P3	2.266 (2)	Pt1—Cl1	2.360 (2)
Pt1—P1	2.359 (2)	Pt1—P2	2.368 (2)
P3—Pt1—P1	98.91 (8)	P3—Pt1—P2	95.87 (8)
P3—Pt1—Cl1	169.58 (10)	P1—Pt1—P2	162.27 (8)
P1—Pt1—Cl1	83.77 (9)	Cl1—Pt1—P2	83.43 (9)

All H atoms were positioned geometrically and treated as riding (C—H = 0.97 Å for methylene and C—H = 0.93 Å otherwise), with $U_{iso}(H) = 1.2U_{eq}(C)$ of the carrier atom. The perchlorate anions are disordered, the site-occupancy factors of the two components being 0.52 (3) and 0.48 (3). The dichloromethane solvent is also disordered, with occupancies of 0.603 (6) and 0.397 (6) for the two components. The highest peak and deepest hole in the final difference map were associated with atom Pt1 (at 0.78 and 1.01 Å, respectively).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (No. 20562007) and Jianxi Provincial Department of Science and Technology.

References

Abram, U., Dell'Amico, D. B., Calderazzo, F., Marchetti, L. & Strahle, J. (1999). *J. Chem. Soc. Dalton Trans.* pp. 4093–4098.

Bruker (1998). *SAINT* (Version 4.00), *SMART* (Version 5.0) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Johansson, M. H. & Otto, S. (2000). *Acta Cryst.* C**56**, e12–e15.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Vogler, A. & Kunkely, H. (2002). *Coord. Chem. Rev.* **230**, 243–251.

m346 Zhang *et al.* • $[PtCl(C_{18}H_{15}P)_3](ClO_4)\cdot 2CH_2Cl_2$ *Acta Cryst.* (2006). E**62**, m345–m346