

Bis(benzyltriphenylphosphonium) tetrachlorido-platinate(II) trichloromethane disolvate

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean $\sigma(C-C)$ = 0.005 Å
R factor = 0.032
wR factor = 0.062
Data-to-parameter ratio = 19.9

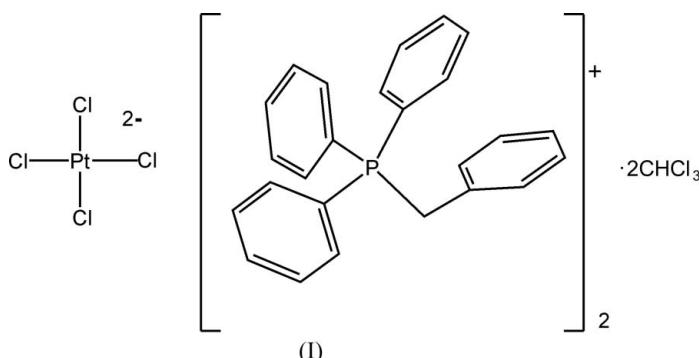
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $(C_{25}H_{22}P)_2[PtCl_4] \cdot 2CHCl_3$, the Pt^{II} atom lies on an inversion centre and the $[PtCl_4]^{2-}$ anion has a square-planar geometry with Pt–Cl bond lengths of 2.3081 (8) and 2.3136 (7) Å. The benzyltriphenylphosphonium cation has a tetrahedral geometry.

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Comment

Complexes $Q_2[PtCl_4]$ with lipophilic cations Q^+ , e.g. $(Ph_3PCH_2Ph)^+$, are used as starting materials for reactions that take place in non-aqueous media, and are important precursors for a wide range of platinum complexes bearing organic ligands.



In the title compound, (I) (Fig. 1), the Pt^{II} atom lies on an inversion centre. The $[PtCl_4]^{2-}$ anion has a square-planar geometry, with Cl–Pt–Cl *cis* angles close to the ideal angle of 90° (Table 1). The Pt–Cl bond lengths [2.3081 (8) and 2.3136 (7) Å] in the anion agree with those found in other $[PtCl_4]^{2-}$ -containing species [2.272 (1)–2.322 (1) Å; Angeloni *et al.*, 2004; Angeloni & Orpen, 2001; Hasan *et al.*, 2001; Ciccarese *et al.*, 1998; Viossat *et al.*, 1994; Lewis & Orpen, 1998; Gillon *et al.*, 2000; Dung *et al.*, 1994; Brammer *et al.*, 1991; Chandrasekaran, 1994; Kao & Chen, 2004; Sakai *et al.*, 1996]. Pt···Pt interactions between the anions are not observed.

In (I), the $(Ph_3PCH_2Ph)^+$ cation has a tetrahedral geometry, with C–P–C angles in the range 106.05 (13)–112.75 (14)°, similar to the conformation found in $(Ph_3PCH_2Ph)_2[Pt_2Cl_6]$ (Kukushkin *et al.*, 1991). The mean planes of the three phenyl P-bonded rings are inclined at 71.42 (15)–77.81 (17)°, forming a propeller-like conformation.

Experimental

Crystals were obtained by recrystallization of $(Ph_3PCH_2Ph)_2[PtCl_4]$ from CHCl₃ at room temperature. Elemental analyses calculated: C 48.70, H 3.62%; found: C 48.67, H 3.60%.

Crystal data



$M_r = 1282.42$

Triclinic, $P\bar{1}$

$a = 9.8900 (3) \text{ \AA}$

$b = 11.2570 (4) \text{ \AA}$

$c = 13.0180 (3) \text{ \AA}$

$\alpha = 98.287 (2)^\circ$

$\beta = 105.042 (2)^\circ$

$\gamma = 108.979 (1)^\circ$

$V = 1281.45 (7) \text{ \AA}^3$

$Z = 1$

Mo $K\alpha$ radiation

$\mu = 3.36 \text{ mm}^{-1}$

$T = 120 (2) \text{ K}$

$0.11 \times 0.10 \times 0.06 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer

Absorption correction: multi-scan
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.717$, $T_{\max} = 0.821$

25993 measured reflections

5866 independent reflections

5484 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.062$

$S = 1.05$

5866 reflections

295 parameters

H-atom parameters constrained

$\Delta\rho_{\max} = 0.86 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.99 \text{ e \AA}^{-3}$

Table 1
Selected geometric parameters (\AA , $^\circ$).

Pt1—Cl1	2.3081 (8)	Pt1—Cl2	2.3126 (7)
Cl1—Pt1—Cl2	89.74 (3)	C9—P1—C21	108.51 (13)
Cl1 ¹ —Pt1—Cl2	90.26 (3)	C15—P1—C2	108.15 (14)
C15—P1—C9	106.05 (13)	C9—P1—C2	110.16 (14)
C15—P1—C21	111.02 (14)	C21—P1—C2	112.75 (14)

Symmetry code: (i) $-x, -y, -z$.

All H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.95–1.00 \AA , and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{parent atom})$.

Data collection: COLLECT (Nonius, 2004); cell refinement: DENZO/SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO/SCALEPACK; program(s) used to solve structure: SIR2004 (Burla *et al.*, 2005); program(s) used to refine structure: SHEXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHEXL97.

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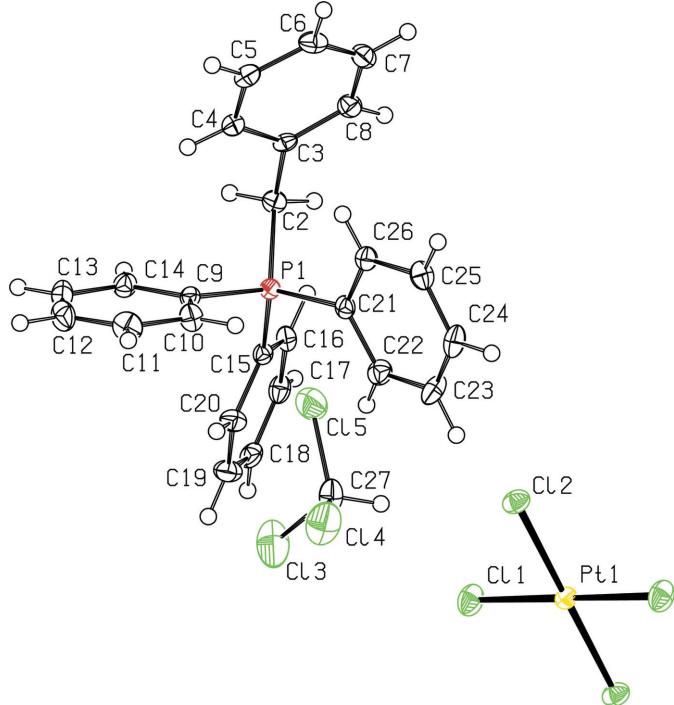


Figure 1

The asymmetric unit of the title compound, showing the atom-labeling scheme. The two symmetry-related Cl atoms are also shown; they are related to the labelled atoms by $(-x, -y, -z)$. Displacement ellipsoids are drawn at the 50% probability level.

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