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Carbonatobis(triphenylphosphine)platinum(II) benzene solvate: a redetermination

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.020 Å
R factor = 0.057
wR factor = 0.126
Data-to-parameter ratio = 14.5

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

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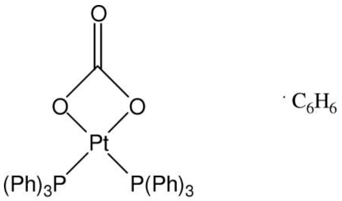
The title compound, $[Pt(CO_3)(C_{18}H_{15}P)_2]\cdot C_6H_6$, has previously been reported by Cariati, Mason, Robertson & Ugo [*Chem. Commun.* (1967), p. 408]. However, no coordinates were published. We present here a redetermination of this structure using new intensity data. The Pt atom shows a distorted square-planar coordination. It carries two PPh_3 residues and is chelated by a carbonate ion.

Comment

Earlier studies have shown that tris(triphenylphosphine)platinum does not react with carbon dioxide in the absence of oxygen; however, in the presence of O_2, a rapid reaction occurs (Nyman *et al.*, 1967). We have found that tetrakis(triphenylphosphine)platinum reacts in C_6D_6 with air to give carbonatobis(triphenylphosphine)platinum(II), (I), as shown in the reaction scheme below.

$$(Ph_3P)_4Pt + CO_2 + O_2 \longrightarrow (Ph_3P)_2PtCO_3 + 2\ Ph_3P$$



(I)

The crystal structure of (I) has already been reported by Cariati *et al.* (1967). However, these authors did not publish any coordinates. We report here the X-ray crystal structure analysis of (I) using new intensity data. A perspective view of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005; *MOGUL* Version 1.0; Allen, 2002). The coordination of the Pt atom is distorted square planar, with an r.m.s. deviation of 0.024 Å for atoms Pt1/P1/P2/O1/O2. The two Pt—O bonds are almost the same length, but the Pt—P bonds differ by 0.037 Å (Table 1). The O atom that is not bonded to Pt shows a significantly shorter C—O bond than the coordinated O atoms. The compound crystallizes with one molecule of benzene in the asymmetric unit.

Experimental

Colourless crystals of the title compound were obtained by storing a solution of $(Ph_3P)_4Pt$ (0.021 g, 0.016 mmol) in C_6D_6 (0.7 ml) in air for several days at room temperature.

Crystal data

$[Pt(CO_3)(C_{18}H_{15}P)_2]\cdot C_6H_6$
$M_r = 857.75$
Triclinic, $P\overline{1}$
$a = 10.594$ (2) Å
$b = 12.512$ (2) Å
$c = 15.195$ (2) Å
$\alpha = 85.15$ (1)°
$\beta = 71.34$ (1)°
$\gamma = 70.91$ (1)°
$V = 1802.9$ (5) Å^3

$Z = 2$
$D_x = 1.580$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12395 reflections
$\theta = 2.1$–25.2°
$\mu = 4.02$ mm^{-1}
$T = 100$ (2) K
Cut needle, colourless
0.11 × 0.08 × 0.04 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)
$T_{\min} = 0.666$, $T_{\max} = 0.856$
21885 measured reflections

6408 independent reflections
4337 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.081$
$\theta_{\max} = 25.2°$
$h = -11 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.126$
$S = 0.95$
6408 reflections
442 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0154P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 2.04$ e Å^{-3}
$\Delta\rho_{\min} = -1.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—O1	2.057 (8)	C1—O3	1.228 (14)
Pt1—O2	2.067 (9)	C1—O2	1.340 (14)
Pt1—P1	2.242 (3)	C1—O1	1.364 (15)
Pt1—P2	2.279 (3)		
O1—Pt1—O2	64.8 (3)	P1—Pt1—P2	98.16 (11)
O1—Pt1—P1	99.7 (3)	O3—C1—O2	124.7 (12)
O2—Pt1—P1	164.2 (2)	O3—C1—O1	125.7 (11)
O1—Pt1—P2	162.1 (2)	O2—C1—O1	109.6 (9)
O2—Pt1—P2	97.3 (2)		

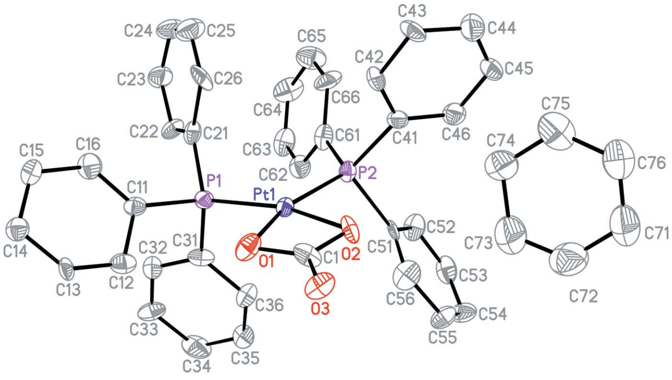


Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted.

All H atoms were included with fixed individual displacement parameters [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)] using a riding model (C—H = 0.95 Å). The largest peak in the differnce Fourier is located 2.01 Å from atom H15. We attribute the unusual displacement ellipsoids of C26 and C51 to an inadequate absorption correction. The deepest hole is located 1.60 Å from atom H72.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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