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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.060
Data-to-parameter ratio = 20.3

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

Triphenylbenzylphosphonium trichloro-(propiononitrile)platinate(II)

In the title platinum(II) propiononitrile complex, [Ph₃PCH₂Ph][PtCl₃(EtCN)], the coordination polyhedron of the metal center is slightly distorted square planar.

Comment

As part of our interest in the reactivity of metal-activated nitriles toward nucleophilic addition (Kukushkin & Pombeiro, 2002), we have performed two kinetic studies devoted to the addition of such HON-nucleophiles as *N,N*-dialkylhydroxy-lamines (Luzyanin *et al.*, 2005) and oximes (Luzyanin *et al.*, 2006) to Pt-bound organonitriles. The known complex [Ph₃PCH₂Ph][PtCl₃(EtCN)], (I), (Kuznetsov *et al.*, 2000) has been chosen as a convenient starting material for these studies because it has only one nitrile ligand, in contrast to the more common [PtCl₂(*R*CN)₂], and can be easily prepared in a pure form. Here we report the molecular structure of (I), determined by a single-crystal X-ray diffraction analysis.

(I)
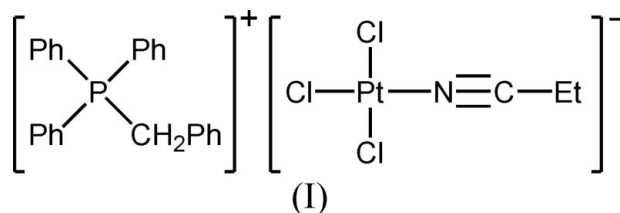
The complex [Ph₃PCH₂Ph][PtCl₃(EtCN)], crystallizes from an acetone solution in air at room temperature in the monoclinic space group $P2_1/c$. In (I), the coordination of the metal center is slightly distorted square planar and the bond lengths and angles (Table 1) are normal (Allen *et al.*, 1987). In the anion, the values of the *trans*-Cl—Pt—Cl bonds and the value of the Pt—Cl bond (*trans* to N) are the same within 3σ, indicating that the ground-state *trans* influence is similar for the nitrile and chloro ligands. The Pt—N and nitrile C≡N bonds are typical for Pt^II–organonitrile complexes (Orpen *et al.*, 1989). In the cation, the P—CH₂ bond is in the range of normal values (1.791–1.841 Å) (Allen *et al.*, 1987). The structure of the title compound is consistent with relevant Pt–organonitrile complexes of the type (cation)[PtCl₃(*R*CN)] with different counter-ions and/or another *R* group in the nitrile (Kukushkin *et al.*, 1990; Wagner *et al.*, 2001).

Experimental

The title complex was prepared according to the method of Kuznetsov *et al.* (2000).

Crystal data

$(C_{25}H_{22}P)[PtCl_3(C_3H_5N)]$
$M_r = 709.92$
Monoclinic, $P2_1/c$
$a = 10.0016 (2)$ Å
$b = 9.0130 (2)$ Å
$c = 30.2234 (6)$ Å
$\beta = 91.7290 (12)°$
$V = 2723.23 (10)$ Å^3

$Z = 4$
$D_x = 1.732$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 5.52$ mm^{-1}
$T = 120 (2)$ K
Plate, yellow
$0.18 \times 0.15 \times 0.08$ mm

Data collection

Nonius KappaCCD diffractometer
φ scans and ω scans with κ offset
Absorption correction: multi-scan
 (SADABS; Sheldrick, 2003)
 $T_{min} = 0.417$, $T_{max} = 0.640$

43536 measured reflections
6249 independent reflections
4944 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.060$
$S = 1.02$
6249 reflections
308 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2 + 2.2335P]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.27$ e Å^{-3}
$\Delta\rho_{min} = -1.25$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pt1—N1	1.976 (4)	P1—C11	1.798 (3)
Pt1—Cl1	2.2822 (10)	P1—C4	1.814 (4)
Pt1—Cl3	2.2997 (9)	N1—C1	1.129 (5)
Pt1—Cl2	2.3069 (9)	C1—C2	1.464 (6)
P1—C23	1.793 (3)	C4—C5	1.510 (5)
P1—C17	1.794 (4)		
N1—Pt1—Cl1	178.41 (9)	C17—P1—C4	108.39 (17)
Cl3—Pt1—Cl2	176.80 (3)	C1—N1—Pt1	178.9 (4)
C23—P1—C11	107.71 (16)	C5—C4—P1	112.0 (2)

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2–1.5U_{eq}(parent atom). The maximum and minimum electron-density peaks lie 1.12 Å from H26 and 0.88 Å from Pt1, respectively.

Data collection: COLLECT (Nonius, 2000); cell refinement: DENZO/SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO/SCALEPACK; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHELXL97.
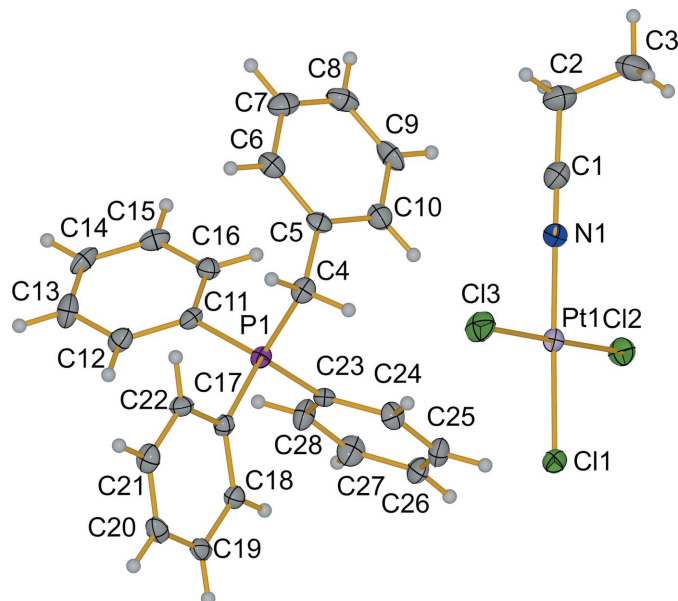
Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

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