trans-Carbonylchloridobis(triethylphosphane-kP)-platinum(II) tetrafluoridoborate

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The chemical formulation of the title compound was established as trans-[PtCl[P(C2H5)3(CO)]BF4 by single-crystal X-ray analysis, in contrast to the five-coordinate tetrafluoroethylene complex that had been anticipated. The compound had been prepared by reaction of trans-PtHCl(P(C2H5)3)2 with C2F4 in the absence of air, and the presence of the carbonyl group was not suspected. The square-planar cations and BF4\(^-\) anions are linked by C—H···F and C—H···O interactions into thick wavy (010) sheets. The present crystal-structure refinement is based on the original intensity data recorded in 1967.

Structure description

A low-yield product in the reaction of trans-PtHCl(P(C2H5)3)2 with C2F4 in the absence of air was originally postulated to be a five-coordinate platinum complex, PtHCl(π-C2F4)(P(C2H5)3)2 (Clark & Tsang, 1967), and the crystal-structure determination was undertaken at that time in view of the then current interest in five-coordination and of π-complexes. As described in Clark *et al.* (1967), the preliminary crystal-structure model showed no evidence of five-coordination, nor of the presence of a π-bonded tetrafluoroethylene group. Instead, a four-coordinated, cationic Pt\(^{II}\) complex was indicated, with a carbonyl group as the fourth ligand, isoelectronic with Vaska’s compound, IrCl(CO)(PR3)2 (Vaska & DiLuzio, 1961). The presence of a carbonyl group was completely unexpected, as the reaction had been carried out in a vacuum line, in the absence of oxygen. This was the first reported molecular structure of a platinum carbonyl at the time, according to our database analysis below. The strong carbonyl vibrational band in the infrared spectrum was mistaken for the anticipated Pt—H band. Evidently, the carbonyl oxygen atom had been extracted from the Pyrex glassware by the tetrafluoroethylene reagent. That reaction vessels are not always as inert as they are expected to be is the subject of a recent review by Nielsen & Pedersen (2022) in which formation of
the title compound in this paper is one of several examples of fluorine compounds reacting with glassware.

The crystal structure refinement based on the original X-ray intensity data recorded in 1967 is now presented here, because no atomic coordinates were given in the original report (Clark et al., 1967) or deposited with the Cambridge Structural Database (CSD; Groom et al., 2016). The square-planar platinum(II) cation and a tetrafluoridoborate anion are shown in Fig. 1. As can be seen, the cation has an approximate mirror plane of symmetry that extends to the conformations of the ethyl groups. The Pt—CO bond length is 1.812 (17) Å, Pt—Cl is 2.301 (4) Å, and the Pt—P bond lengths are 2.341 (5) and 2.348 (5) Å. The P—Pt—CO angles average 92.9 (8)° while the Cl—Pt—P angles average 87.2 (2)°. The trans angles P—Pt—P and Cl—Pt—C are 174.10 (17)° and 177.0 (12)°, respectively, with the slight distortions from linearity tending towards a flattened tetrahedron rather than a flattened square pyramid. Each of the triethylphosphine groups has one ethyl group in the trans conformation and two in the gauche conformation.

Packing diagrams showing views down the b and c axes are shown in Fig. 2a and 2b. There are close contacts between each tetrafluoridoborate anion and the ethyl groups of three neighboring cations with putative C—H···F hydrogen bonds, as listed in Table 1. The Hirshfeld $d_{\text{norm}}$ plot for the BF$_4^-$ anion shown in Fig. 3 was produced with CrystalExplorer (Spackman et al., 2021) and indicates a close contact near F2, probably due to the C13—H13···F2 hydrogen bond, which seems to be the strongest C—H···F bond. The chlorido and carbonyl ligands do not have close intermolecular contacts, perhaps because they are shielded by the gauche conformations of the neighboring ethyl groups. A putative weak C—H···O hydrogen bond is listed in Table 1 and shown in red in Fig. 3. The hydrogen bonds listed join cations and anions into thick wavy (010) sheets, as can be seen in Fig. 2b.

**Database analysis**

From the time the preliminary structure of this compound was published in 1967, crystal and molecular structures of a

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**Table 1**

| $D-H \cdot A$ | $D-H$ | $H \cdot A$ | $D-A$ | $D-H \cdot A$ |
|--------------|-------|------------|-------|--------------|
| C5—H5B···O1' | 0.97  | 2.75       | 3.45 (2) | 129          |
| C13—H13B···F2" | 0.96 | 2.43       | 3.27 (3) | 147          |
| C4—H4A···F2   | 0.97  | 2.56       | 3.48 (3) | 159          |
| C7—H7A···F4mm | 0.97 | 2.67       | 3.46 (3) | 140          |
| C11—H11B···F3  | 0.96 | 2.75       | 3.47 (3) | 133          |
| C6—H6A···F1m   | 0.97 | 2.81       | 3.67 (4) | 147          |

Symmetry codes: (i) $x, -y+1, z$; (ii) $-x, y, z + \frac{1}{2}$; (iii) $-x, -y+1, z + \frac{1}{2}$.
wide variety of platinum carbonyl complexes have been reported, ranging from metal clusters through monomeric complexes as in this case. All 662 structures found with the ‘PtCO’ search fragment in the CSD database, with all filters removed except for ‘single-crystal structure’, except the present one (TEPPTC) are dated 1968 or after. All but 20 of these structures have only one CO group coordinating to the PtII atom while the rest have just two coordinating carbonyl groups except for the [Pt(CO)4]2+ cation reported by Willner et al. (2001) in entry QEZTEU. The mean Pt—CO distance for the 603 structures with coordinates given is 1.860 Å, with a wide range of 1.680 to 2.095 Å. It is interesting that the presence of phosphine ligands tends to lead to longer Pt—CO distances, while the presence of a Cl ligand to shorter Pt—CO distances. Thus, in the 35 entries in the above structures that have two PR3 groups attached to the PtII atom as well as the CO group, the mean Pt—C distance is 1.910 Å, with a narrow range of 1.855–1.965 Å, while for the 36 entries that have a Cl as well as a carbonyl ligand, the mean Pt—CO distance is 1.837 Å with a range of 1.753 to 1.901 Å. In the latter case, the Pt—CO distance seems insensitive to whether the Cl atom is cis or trans to the CO group. These tendencies must oppose each other in the present structure, leading to the Pt—CO distance of 1.812 (17) Å. Entry GEYBOB (Rusakov et al., 1988) has the same cation as in the present structure, leading to the Pt—CO distance of 1.837 Å with a range of 1.753 to 1.901 Å. In the latter case, the Pt—CO bond length of 1.846 Å.

Synthesis and crystallization

A sample supplied by Dr H. C. Clark had been synthesized as described in Clark & Tsang (1967). Crystals suitable for X-ray analysis were obtained by recrystallization of the sample from methyl acetate.

Refinement

With the early automatic diffractometer that was used to collect the original X-ray intensity data in 1967, it was not customary to obtain a set of Friedel pairs of reflections in the case of a non-centrosymmetric structure. In this case, however, due to the polar space group and the poor scattering by the small crystal, data were collected over the whole sphere of reflection up to θ = 20°; in addition, data were recollected over four quadrants for the weaker reflections at higher angles. Initial absorption corrections using a Gaussian grid were inconclusive – perhaps due to a programming error –, so for the final refinements an overall absorption correction using the tensor analysis in XABS2 (Parkin et al., 1995) was used. Hydrogen atoms were constrained, with C—H distances of 0.97 Å and 0.96 Å for CH2 and CH3 groups, respectively, and $U_{iso}(H) = 1.5U_{eq}(C)$. Anisotropic temperature factors for the carbonyl CO atoms required tight restraints. While the displacement ellipsoids for the fluorine atoms are large, probably indicating some disorder for the BF4− anion (Fig. 1), initial refinements of a disordered model were not successful and the disordered model was not pursued. There is indeed some residual electron density in the neighborhood of the BF4− anion, but only one of the 20 highest electron density peaks in the final difference-Fourier map is near this group. Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

I am deeply grateful to the late James A. Ibers, who suggested this problem and submitted the earlier communication on the present one (TEPPTC), except the 20 highest electron density peaks in the final difference-Fourier map is near this group. Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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Clark, H. C. & Tsang, W. S. (1967). J. Am. Chem. Soc. 89, 529–533.

Table 2

| Crystal data                          | [PtCl(C6H15P)2(CO)]BF4 |
|--------------------------------------|------------------------|
| Chemical formula                     | [PtCl(C6H15P)2(CO)]BF4 |
| M₀                                   | 581.66                 |
| Crystal system, space group          | Orthorhombic, Pca2₁    |
| Temperature (K)                      | 293                    |
| a, b, c (Å)                          | 16.012 (8), 9.171 (4), 14.966 (7) |
| V (Å³)                               | 21977.1 (18)           |
| Z                                     | 4                      |
| Radiation type                       | Mo Kα                  |
| μ (mm⁻¹)                             | 6.68                   |
| Crystal size (mm)                    | 0.12 x 0.10 x 0.08     |

Data collection

| Diffractometer                       | Picker, punched card control |
|--------------------------------------|-------------------------------|
| Absorption correction                | Empirical (using intensity measurements) (XABS2; Parkin et al., 1995) |
| T_min, T_max                         | 0.55, 0.81                   |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 7773, 3180, 2437 |
| R_max (sin θ/λ)max (Å⁻¹)             | 0.062                        |
| Absolute structure                   | Flack x determined using 961 quotations [(I)−(I')]/[(I)+(I')] (Parsons et al., 2013) |
| Absolute structure parameter         | 0.000 (14)                   |

Computer programs: PICK (local program by J. A. Ibers), PICKOUT (local program by R. J. Doedens) and EQUIV (local program by J. A. Ibers), local version of FORDAP, SHELXL (Sheldrick, 2015), ORTEPIII (Burnett & Johnson, 1996; Farrugia, 2012) and pubICIF (Westrip, 2010).
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Crystal data

\[
\begin{align*}
\text{[PtCl(C_6H_{15}P)_2(CO)]BF}_4 \\
M_r &= 581.66 \\
\text{Orthorhombic, } Pca2_1 \\
a &= 16.012 (8) \text{ Å} \\
b &= 9.171 (4) \text{ Å} \\
c &= 14.966 (7) \text{ Å} \\
V &= 2197.7 (18) \text{ Å}^3 \\
Z &= 4 \\
F(000) &= 1128
\end{align*}
\]

\[D_s = 1.758 \text{ Mg m}^{-3}\]

\[D_m = 1.734 (4) \text{ Mg m}^{-3}\]

\[D_m \text{ measured by flotation in CH}_3\text{I/CCl}_4\]

Mo Kα radiation, \(\lambda = 0.7107 \text{ Å}\)

Cell parameters from 16 reflections

\[\theta = 3.7–14.1^\circ\]

\[\mu = 6.68 \text{ mm}^{-1}\]

\[T = 293 \text{ K}\]

Needle, colorless

0.12 × 0.10 × 0.08 mm

Data collection

Picker, punched card control diffractometer

Radiation source: sealed X-ray tube

\(\theta/2\theta\) scans

Absorption correction: empirical (using intensity measurements)

\((XABS2; \text{Parkin et al., 1995})\)

\(T_{\text{min}} = 0.55, T_{\text{max}} = 0.81\)

7773 measured reflections

3180 independent reflections

2437 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.062\)

\(\theta_{\text{max}} = 25.1^\circ, \theta_{\text{min}} = 2.2^\circ\)

\(h = 0\to 19\)

\(k = 0\to 10\)

\(l = -17\to 17\)

3 standard reflections every 250 reflections

intensity decay: 8(2)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R(F^2 > 2\sigma(F^2)) = 0.041\)

\(wR(F^2) = 0.090\)

\(S = 0.92\)

3180 reflections

214 parameters

61 restraints

Primary atom site location: heavy-atom method

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\(w = 1/[\sigma^2(F_c^2)]\)

where \(P = (F_c^2 + 2F_s^2)/3\)

\((\Delta\sigma)_{\text{max}} = 0.002\)

\(\Delta\rho_{\text{max}} = 0.64 \text{ e Å}^{-3}\)

\(\Delta\rho_{\text{min}} = -0.76 \text{ e Å}^{-3}\)

Absolute structure: Flack \(x\) determined using 961 quotients \([I^-)-(I^+)/[I^-]+(I^+)\) (Parsons et al., 2013)

Absolute structure parameter: 0.000 (14)
**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

|   | x      | y      | z      | Uiso/Ueq |
|---|--------|--------|--------|----------|
| Pt| 0.1189 (3) | 0.19055 (6) | 0.49793 (9) | 0.0540 (2) |
| CL| 0.0065 (3) | 0.0347 (5) | 0.5053 (8) | 0.0837 (17) |
| P1| 0.1894 (3) | 0.0057 (5) | 0.4207 (4) | 0.0580 (13) |
| P2| 0.0355 (3) | 0.3627 (6) | 0.5723 (3) | 0.0606 (14) |
| C1| 0.2098 (10) | 0.3084 (18) | 0.497 (3) | 0.074 (5) |
| C2| 0.2670 (8) | 0.3789 (15) | 0.498 (2) | 0.114 (5) |
| H2A| 0.138889 | −0.191260 | 0.502025 | 0.102* |
| H2B| 0.120055 | −0.236749 | 0.450938 | 0.102* |
| C3| 0.1344 (12) | −0.048 (2) | 0.3209 (13) | 0.081 (6) |
| H3A| 0.167832 | −0.120101 | 0.289379 | 0.122* |
| H3B| 0.082483 | −0.095089 | 0.338078 | 0.122* |
| C4| 0.2941 (10) | 0.045 (2) | 0.3857 (11) | 0.061 (5) |
| H4A| 0.293095 | 0.132343 | 0.349114 | 0.092* |
| H4B| 0.327255 | 0.066627 | 0.438343 | 0.092* |
| C5| −0.0571 (12) | 0.405 (2) | 0.510 (2) | 0.089 (7) |
| H5A| −0.087502 | 0.315295 | 0.499106 | 0.133* |
| H5B| −0.092341 | 0.467457 | 0.545982 | 0.133* |
| C6| 0.0892 (12) | 0.5313 (19) | 0.5972 (14) | 0.071 (6) |
| H6A| 0.136834 | 0.509449 | 0.634974 | 0.107* |
| H6B| 0.110475 | 0.571661 | 0.541807 | 0.107* |
| C7| −0.0026 (13) | 0.295 (2) | 0.6757 (12) | 0.074 (6) |
| H7A| −0.035167 | 0.370900 | 0.704742 | 0.111* |
| C8| 0.2499 (16) | 0.213328 | 0.664405 | 0.111* |
| C9| 0.1148 (15) | 0.076 (3) | 0.2576 (15) | 0.117 (9) |
| H9A| 0.087111 | 0.039006 | 0.205509 | 0.175* |
| H9B| 0.165842 | 0.123467 | 0.240124 | 0.175* |
| C10| 0.145449 | 0.3335 (15) | 0.095 (7) |
| H10A| 0.394947 | −0.048653 | 0.323932 | 0.143* |
| H10B| 0.310361 | −0.087509 | 0.276862 | 0.143* |
| C11| −0.042045 | 0.377 (3) | 0.4237 (19) | 0.141 (12) |
| H11A| −0.093656 | 0.471759 | 0.388736 | 0.212* |
| H11B| 0.001072 | 0.428995 | 0.392480 | 0.212* |
| Atom  | u_{11} (Å²) | u_{22} (Å²) | u_{33} (Å²) | u_{12} (Å²) | u_{13} (Å²) | u_{23} (Å²) |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|
| Pt    | 0.0466 (3)  | 0.0576 (3)  | 0.0578 (3)  | −0.0066 (3) | −0.0007 (10)| 0.0042 (9)  |
| C1    | 0.051 (3)   | 0.067 (3)   | 0.057 (3)   | −0.003 (3)  | 0.000 (3)   | 0.006 (3)   |
| C2    | 0.083 (11)  | 0.066 (11)  | 0.055 (13)  | 0.012 (13)  | −0.037 (12) | −0.013 (11) |
| C3    | 0.083 (15)  | 0.083 (14)  | 0.078 (14)  | 0.012 (13)  | −0.037 (12) | −0.013 (11) |
| C4    | 0.049 (11)  | 0.080 (12)  | 0.055 (12)  | −0.007 (10) | 0.009 (9)   | −0.003 (10) |
| C5    | 0.091 (13)  | 0.097 (14)  | 0.079 (18)  | 0.032 (11)  | −0.012 (16) | 0.022 (16)  |
| C6    | 0.078 (14)  | 0.059 (12)  | 0.077 (15)  | −0.020 (10) | 0.034 (11)  | 0.001 (10)  |
| C7    | 0.084 (13)  | 0.078 (14)  | 0.060 (12)  | 0.015 (12)  | 0.035 (9)   | 0.025 (12)  |
| C8    | 0.122 (19)  | 0.105 (18)  | 0.072 (14)  | 0.003 (16)  | −0.009 (13) | 0.035 (13)  |
| C9    | 0.16 (2)    | 0.106 (18)  | 0.082 (16)  | 0.038 (17)  | −0.057 (16) | −0.005 (13) |
| C10   | 0.099 (17)  | 0.081 (15)  | 0.105 (17)  | 0.021 (13)  | 0.019 (13)  | −0.007 (13) |
| C11   | 0.102 (19)  | 0.22 (3)    | 0.102 (19)  | 0.05 (2)    | −0.014 (16) | 0.08 (2)    |
| C12   | 0.13 (2)    | 0.077 (16)  | 0.12 (2)    | 0.016 (14)  | 0.062 (17)  | 0.017 (14)  |
| C13   | 0.110 (17)  | 0.12 (2)    | 0.066 (14)  | 0.001 (16)  | 0.002 (12)  | 0.026 (14)  |
| B     | 0.061 (13)  | 0.044 (13)  | 0.087 (17)  | −0.012 (11) | −0.011 (13) | −0.006 (13) |
| F1    | 0.37 (4)    | 0.19 (2)    | 0.30 (4)    | −0.11 (3)   | 0.10 (3)    | −0.08 (2)   |
| F2    | 0.189 (18)  | 0.128 (13)  | 0.22 (2)    | 0.060 (15)  | −0.006 (19) | 0.034 (14)  |
| F3    | 0.18 (2)    | 0.38 (4)    | 0.24 (3)    | 0.07 (2)    | 0.123 (19)  | 0.13 (2)    |
| F4    | 0.25 (3)    | 0.39 (4)    | 0.20 (2)    | 0.14 (3)    | −0.08 (2)   | −0.04 (2)   |

**Geometric parameters (Å, °)**

| Bond        | Length (Å) | Angle (°) |
|-------------|------------|-----------|
| Pt—C1       | 1.813 (18) | C7—C13    | 1.56 (3)  |
| Pt—CL       | 2.301 (4)  | C7—H7A    | 0.970     |
| Pt—P1       | 2.341 (5)  | C7—H7B    | 0.970     |
| Pt—P2       | 2.348 (5)  | C8—H8A    | 0.960     |
P1—C2 1.812 (17) C8—H8B 0.9600
P1—C3 1.804 (18) C8—H8C 0.9600
P1—C4 1.794 (16) C9—H9A 0.9600
P2—C5 1.80 (2) C9—H9B 0.9600
P2—C6 1.808 (18) C9—H9C 0.9600
P2—C7 1.775 (17) C10—H10A 0.9600
C1—O1 1.120 (17) C10—H10B 0.9600
C2—C8 1.50 (3) C10—H10C 0.9600
C2—H2A 0.9700 C11—H11A 0.9600
C2—H2B 0.9700 C11—H11B 0.9600
C3—C9 1.52 (3) C11—H11C 0.9600
C3—H3A 0.9700 C12—H12A 0.9600
C3—H3B 0.9700 C12—H12B 0.9600
C4—C10 1.52 (2) C12—H12C 0.9600
C4—H4A 0.9700 C13—H13A 0.9600
C4—H4B 0.9700 C13—H13B 0.9600
C5—C11 1.46 (4) C13—H13C 0.9600
C5—H5A 0.9700 B—F1 1.21 (3)
C5—H5B 0.9700 B—F2 1.25 (3)
C6—C12 1.51 (2) B—F3 1.30 (3)
C6—H6A 0.9700 B—F4 1.20 (3)
C6—H6B 0.9700

C1—Pt—CL 177.0 (12) C12—C6—H6A 108.5
C1—Pt—P1 92.4 (8) C12—C6—H6B 108.5
C1—Pt—P2 93.3 (8) H6A—C6—H6B 107.5
CL—Pt—P1 87.2 (2) C13—C7—H7A 109.0
CL—Pt—P2 87.1 (2) C13—C7—H7B 109.0
P1—Pt—P2 174.10 (17) H7A—C7—H7B 107.8
O1—C1—Pt 178 (3) C2—C8—H8A 109.5
C2—P1—Pt 111.4 (8) C2—C8—H8B 109.5
C3—P1—Pt 111.9 (7) C2—C8—H8C 109.5
C4—P1—Pt 116.7 (6) H8A—C8—H8B 109.5
C2—P1—C4 106.4 (9) H8A—C8—H8C 109.5
C2—P1—C3 103.9 (11) H8B—C8—H8C 109.5
C3—P1—C4 105.6 (10) C3—C9—H9A 109.5
C5—P2—Pt 111.5 (10) C3—C9—H9B 109.5
C6—P2—Pt 113.7 (6) C3—C9—H9C 109.5
C7—P2—Pt 112.0 (7) C9—H9A—C9—H9B 109.5
C5—P2—C6 108.3 (10) H9A—C9—H9C 109.5
C5—P2—C7 104.3 (12) H9B—C9—H9C 109.5
C6—P2—C7 106.4 (10) C4—C10—H10A 109.5
P1—C2—C8 110.5 (14) C4—C10—H10B 109.5
P1—C3—C9 114.2 (16) C4—C10—H10C 109.5
P1—C4—C10 115.7 (14) H10A—C10—H10B 109.5
P2—C5—C11 115.7 (17) H10A—C10—H10C 109.5
P2—C6—C12 115.1 (14) H10B—C10—H10C 109.5
P2—C7—C13 112.8 (14) C5—C11—H11A 109.5
Hydrogen-bond geometry (Å, º)

| D—H···A  | D—H  | H···A  | D···A  | D—H···A |
|----------|------|--------|--------|---------|
| C5—H5B···O1i | 0.97 | 2.75   | 3.45 (2) | 129     |
| C13—H13B···F2ii | 0.96 | 2.43   | 3.27 (3) | 147     |
| C4—H4A···F2    | 0.97 | 2.56   | 3.48 (3) | 159     |
| C7—H7A···F4iii | 0.97 | 2.67   | 3.46 (3) | 140     |
| C11—H11B···F3  | 0.96 | 2.75   | 3.47 (3) | 133     |
| C6—H6A···F11i  | 0.97 | 2.81   | 3.67 (4) | 147     |

Symmetry codes: (i) x-1/2, -y+1, z; (ii) -x+1/2, y, z+1/2; (iii) -x, -y+1, z+1/2.