

cis-Dichloridobis(triphenylphosphine- κP)platinum(II) chloroform solvate

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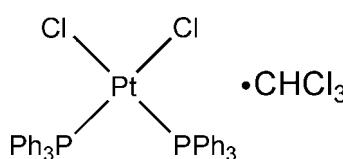
Received 21 July 2009; accepted 28 July 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.013$ Å; disorder in solvent or counterion; R factor = 0.048; wR factor = 0.119; data-to-parameter ratio = 15.8.

In the title compound, $[PtCl_2(C_{18}H_{15}P)_2] \cdot CHCl_3$, each Pt^{II} centre adopts a nearly square-planar coordination geometry formed by two P atoms [Pt–P = 2.2481 (17) and 2.2658 (19) Å] and two Cl anions [Pt–Cl = 2.3244 (19) and 2.3548 (17) Å]. The Cl atoms of the chloroform solvent molecule are disordered over two orientations in a 0.778 (11):0.222 (11) ratio. The crystal packing is stabilized by weak intermolecular C–H···Cl hydrogen bonds, exhibiting voids with a volume of 215 Å³.

Related literature

For the preparation of *cis*-[PtCl₂(PPh₃)₂], see: Bailar & Itatani (1965). For the structure of *trans*-[PtCl₂(PPh₃)₂], see: Johansson & Otto (2000). For the structures of related *cis*-complexes, see: Anderson *et al.* (1982); Al-Fawaz *et al.* (2004); Fun *et al.* (2006).



Experimental

Crystal data

$[PtCl_2(C_{18}H_{15}P)_2] \cdot CHCl_3$

$M_r = 909.90$

Monoclinic, $P2_1/c$
 $a = 10.3174$ (9) Å
 $b = 24.436$ (2) Å
 $c = 15.6298$ (18) Å
 $\beta = 98.199$ (1) $^\circ$
 $V = 3900.3$ (7) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 4.05$ mm⁻¹
 $T = 298$ K
 $0.38 \times 0.35 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
 $T_{\min} = 0.309$, $T_{\max} = 0.530$
(expected range = 0.281–0.483)

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.119$
 $S = 0.97$
6877 reflections

434 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.89$ e Å⁻³
 $\Delta\rho_{\min} = -1.27$ e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|-----------------------------|-------|--------------|--------------|----------------|
| C3—H3···Cl1 ⁱ | 0.93 | 2.80 | 3.670 (10) | 157 |
| C37—H37···Cl2 ⁱⁱ | 0.98 | 2.43 | 3.390 (15) | 165 |

Symmetry codes: (i) $x + 1, y, z$; (ii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the University of Jinan (grant No. B0605) and the Key Subject Research Foundation of Shandong Province (grant No. XTD 0704) for support of this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2593).

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supplementary materials

Acta Cryst. (2009). E65, m1025 [doi:10.1107/S1600536809029961]

cis-Dichloridobis(triphenylphosphine- κP)platinum(II) chloroform solvate

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Comment

cis- and *trans*-Dichloridobis (triphenylphosphine)platinum(II) are useful to prepare other platinum complexes. The structures of the *cis*-isomer, either in unsolvated form (Fun *et al.*, 2006) or as an acetone (Anderson *et al.*, 1982) or trichloroform solvate (Al-Fawaz *et al.*, 2004) have been reported. During the course of our studies on platinaborane cluster compounds using the *cis*-isomer as a starting material, we unexpectedly obtained the yellowish crystals of the title compound (I).

As shown in Fig.1, the platinum centre is four-coordinated and adopts a nearly square planar geometry. The Pt—P bond lengths (2.2481 (17) and 2.2658 (19) Å) and Pt—Cl bond lengths (2.3244 (19) and 2.3548 (17) Å), as well as the bond angles around the Pt atom are similar to those in the above-mentioned structures.

Intermolecular C—H···Cl hydrogen bonding is observed between the chloroform and the chloride (Table 1). Moreover, similar C—H···Cl interaction between one of the phenyl groups and the chloride (Table 1) links the molecules into a one-dimensional chain structure.

Experimental

A mixture of $\text{PtCl}_2(\text{PPh}_3)_2$ (314 mg, 0.4 mmol) and $(\text{Et}_4\text{N})_2\text{B}_{10}\text{H}_{10}$ (150 mg, 0.4 mmol) in $\text{HOCH}_2\text{CH}_2\text{OH}$ (38 ml) was heated at 100°C (oil) under N_2 atmosphere for 39 h. The resulting mixture was filtered to get a red filtrate, to which *ca* 400 ml of water was added. The lower layer formed was separated and treated with water. This process was repeated till the lower layer was colourless. The upper water phase combined was extracted with CH_2Cl_2 . The yellow organic layer was dried to result in a reddish solid. Recrystallization in CHCl_3/n -hexane(1:4, *V*: *V*) afforded a small amount of yellowish crystals of the title compound suitable for X-ray analysis.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with $d(\text{C}—\text{H}) = 0.93$ Å, $U_{\text{iso}}=1.2U_{\text{eq}}$ (C) for aromatic, and $d(\text{C}—\text{H}) = 0.98$ Å, $U_{\text{iso}}=1.5U_{\text{eq}}$ (C) for CHCl_3 . The highest residual peak [$1.89 \text{ e}\text{\AA}^{-3}$] and deepest hole [$-1.27 \text{ e}\text{\AA}^{-3}$] are situated 1.05 Å and 0.97 Å, respectively, at atom Pt1.

supplementary materials

Figures

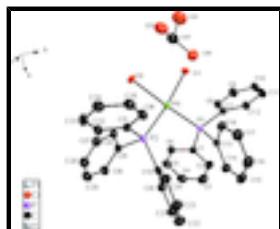


Fig. 1. View of (I) with atom labels and 25% probability displacement ellipsoids. For the disordered chloroform molecule, only major part is shown for clarity.

cis-Dichloridobis(triphenylphosphine- κP)platinum(II) chloroform solvate

Crystal data

| | |
|---|---|
| [PtCl ₂ (C ₁₈ H ₁₅ P) ₂]·CHCl ₃ | $F_{000} = 1784$ |
| $M_r = 909.90$ | $D_x = 1.550 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 10.3174 (9) \text{ \AA}$ | Cell parameters from 8493 reflections |
| $b = 24.436 (2) \text{ \AA}$ | $\theta = 2.2\text{--}28.2^\circ$ |
| $c = 15.6298 (18) \text{ \AA}$ | $\mu = 4.05 \text{ mm}^{-1}$ |
| $\beta = 98.1990 (10)^\circ$ | $T = 298 \text{ K}$ |
| $V = 3900.3 (7) \text{ \AA}^3$ | Block, yellowish |
| $Z = 4$ | $0.38 \times 0.35 \times 0.18 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker SMART CCD area-detector diffractometer | 6877 independent reflections |
| Radiation source: fine-focus sealed tube | 4984 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.071$ |
| $T = 298 \text{ K}$ | $\theta_{\text{max}} = 25.0^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 1.6^\circ$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2001) | $h = -12 \rightarrow 12$ |
| $T_{\text{min}} = 0.309$, $T_{\text{max}} = 0.530$ | $k = -29 \rightarrow 28$ |
| 18772 measured reflections | $l = -14 \rightarrow 18$ |

Refinement

| | |
|---------------------------------|---|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H-atom parameters constrained |
| $wR(F^2) = 0.119$ | $w = 1/[\sigma^2(F_o^2) + (0.0594P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.97$ | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 6877 reflections | $\Delta\rho_{\text{max}} = 1.89 \text{ e \AA}^{-3}$ |

434 parameters

$$\Delta\rho_{\min} = -1.27 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct
methods Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|--------------|---------------|---------------|----------------------------------|------------|
| Pt1 | 0.59334 (2) | 0.349888 (10) | 0.548206 (18) | 0.03195 (11) | |
| Cl1 | 0.45377 (18) | 0.39079 (8) | 0.43652 (13) | 0.0477 (5) | |
| Cl2 | 0.41302 (18) | 0.29552 (8) | 0.57114 (13) | 0.0492 (5) | |
| Cl3 | 0.2158 (6) | 0.3208 (3) | 0.2316 (4) | 0.142 (3) | 0.778 (11) |
| Cl4 | 0.1897 (12) | 0.3400 (5) | 0.0514 (7) | 0.165 (4) | 0.778 (11) |
| Cl5 | 0.4219 (6) | 0.3691 (2) | 0.1644 (6) | 0.141 (3) | 0.778 (11) |
| Cl3' | 0.355 (3) | 0.3779 (12) | 0.078 (2) | 0.197 (14) | 0.222 (11) |
| Cl4' | 0.348 (3) | 0.3554 (9) | 0.2339 (17) | 0.156 (12) | 0.222 (11) |
| Cl5' | 0.147 (4) | 0.3153 (17) | 0.081 (3) | 0.167 (13) | 0.222 (11) |
| P1 | 0.75776 (17) | 0.40376 (7) | 0.51837 (12) | 0.0316 (4) | |
| P2 | 0.70533 (18) | 0.30561 (7) | 0.66301 (13) | 0.0359 (4) | |
| C1 | 0.8924 (7) | 0.3665 (3) | 0.4836 (5) | 0.0416 (18) | |
| C2 | 1.0068 (7) | 0.3918 (4) | 0.4670 (6) | 0.054 (2) | |
| H2 | 1.0160 | 0.4295 | 0.4733 | 0.065* | |
| C3 | 1.1060 (9) | 0.3615 (4) | 0.4413 (7) | 0.072 (3) | |
| H3 | 1.1836 | 0.3786 | 0.4326 | 0.086* | |
| C4 | 1.0925 (9) | 0.3063 (4) | 0.4282 (6) | 0.068 (3) | |
| H4 | 1.1614 | 0.2861 | 0.4120 | 0.081* | |
| C5 | 0.9789 (8) | 0.2810 (4) | 0.4387 (6) | 0.061 (2) | |
| H5 | 0.9677 | 0.2439 | 0.4264 | 0.074* | |
| C6 | 0.8797 (8) | 0.3107 (3) | 0.4677 (5) | 0.048 (2) | |
| H6 | 0.8030 | 0.2930 | 0.4767 | 0.058* | |
| C7 | 0.7173 (7) | 0.4505 (3) | 0.4270 (5) | 0.0400 (18) | |
| C8 | 0.7002 (8) | 0.4296 (3) | 0.3447 (5) | 0.051 (2) | |
| H8 | 0.7101 | 0.3922 | 0.3367 | 0.061* | |
| C9 | 0.6684 (9) | 0.4631 (4) | 0.2731 (6) | 0.065 (3) | |
| H9 | 0.6554 | 0.4486 | 0.2175 | 0.078* | |
| C10 | 0.6564 (8) | 0.5200 (4) | 0.2873 (6) | 0.061 (2) | |
| H10 | 0.6362 | 0.5433 | 0.2403 | 0.073* | |
| C11 | 0.6737 (8) | 0.5407 (4) | 0.3678 (6) | 0.058 (2) | |
| H11 | 0.6650 | 0.5782 | 0.3760 | 0.070* | |
| C12 | 0.7044 (7) | 0.5067 (3) | 0.4382 (5) | 0.048 (2) | |
| H12 | 0.7165 | 0.5214 | 0.4936 | 0.058* | |
| C13 | 0.8127 (7) | 0.4487 (3) | 0.6099 (5) | 0.0394 (17) | |
| C14 | 0.9418 (8) | 0.4603 (3) | 0.6409 (5) | 0.053 (2) | |
| H14 | 1.0093 | 0.4437 | 0.6168 | 0.064* | |
| C15 | 0.9694 (10) | 0.4972 (4) | 0.7088 (6) | 0.067 (3) | |
| H15 | 1.0560 | 0.5044 | 0.7317 | 0.080* | |
| C16 | 0.8705 (10) | 0.5230 (4) | 0.7418 (7) | 0.070 (3) | |
| H16 | 0.8902 | 0.5487 | 0.7857 | 0.084* | |
| C17 | 0.7427 (10) | 0.5116 (3) | 0.7111 (6) | 0.065 (3) | |

supplementary materials

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|-----|-------------|------------|------------|-------------|
| H17 | 0.6756 | 0.5288 | 0.7347 | 0.078* |
| C18 | 0.7138 (8) | 0.4744 (3) | 0.6452 (5) | 0.050 (2) |
| H18 | 0.6268 | 0.4666 | 0.6242 | 0.061* |
| C19 | 0.8622 (7) | 0.3305 (3) | 0.7180 (5) | 0.046 (2) |
| C20 | 0.9782 (8) | 0.3178 (3) | 0.6859 (6) | 0.054 (2) |
| H20 | 0.9755 | 0.2978 | 0.6351 | 0.065* |
| C21 | 1.0977 (9) | 0.3351 (4) | 0.7302 (7) | 0.066 (3) |
| H21 | 1.1753 | 0.3261 | 0.7097 | 0.079* |
| C22 | 1.1006 (10) | 0.3649 (4) | 0.8029 (8) | 0.074 (3) |
| H22 | 1.1808 | 0.3771 | 0.8312 | 0.088* |
| C23 | 0.9906 (10) | 0.3775 (4) | 0.8358 (7) | 0.072 (3) |
| H23 | 0.9962 | 0.3974 | 0.8870 | 0.086* |
| C24 | 0.8702 (9) | 0.3613 (3) | 0.7945 (6) | 0.056 (2) |
| H24 | 0.7945 | 0.3706 | 0.8170 | 0.067* |
| C25 | 0.7459 (7) | 0.2350 (3) | 0.6415 (5) | 0.0449 (19) |
| C26 | 0.6929 (8) | 0.2102 (3) | 0.5647 (6) | 0.053 (2) |
| H26 | 0.6354 | 0.2294 | 0.5242 | 0.063* |
| C27 | 0.7260 (10) | 0.1560 (4) | 0.5481 (7) | 0.072 (3) |
| H27 | 0.6905 | 0.1390 | 0.4969 | 0.086* |
| C28 | 0.8114 (10) | 0.1285 (4) | 0.6082 (8) | 0.075 (3) |
| H28 | 0.8359 | 0.0929 | 0.5965 | 0.090* |
| C29 | 0.8601 (10) | 0.1517 (4) | 0.6835 (8) | 0.073 (3) |
| H29 | 0.9149 | 0.1316 | 0.7243 | 0.088* |
| C30 | 0.8301 (8) | 0.2050 (3) | 0.7013 (6) | 0.057 (2) |
| H30 | 0.8662 | 0.2210 | 0.7533 | 0.069* |
| C31 | 0.6018 (7) | 0.3029 (3) | 0.7490 (5) | 0.0418 (18) |
| C32 | 0.5768 (7) | 0.2541 (3) | 0.7894 (5) | 0.053 (2) |
| H32 | 0.6147 | 0.2217 | 0.7739 | 0.064* |
| C33 | 0.4960 (8) | 0.2537 (4) | 0.8523 (5) | 0.059 (2) |
| H33 | 0.4781 | 0.2208 | 0.8782 | 0.071* |
| C34 | 0.4418 (8) | 0.3009 (4) | 0.8770 (6) | 0.062 (2) |
| H34 | 0.3872 | 0.3006 | 0.9195 | 0.074* |
| C35 | 0.4694 (9) | 0.3492 (4) | 0.8379 (6) | 0.058 (2) |
| H35 | 0.4350 | 0.3819 | 0.8555 | 0.069* |
| C36 | 0.5457 (8) | 0.3501 (3) | 0.7742 (6) | 0.054 (2) |
| H36 | 0.5603 | 0.3830 | 0.7473 | 0.065* |
| C37 | 0.2974 (13) | 0.3240 (6) | 0.1404 (9) | 0.106 (4) |
| H37 | 0.3347 | 0.2879 | 0.1316 | 0.127* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|--------------|
| Pt1 | 0.02648 (17) | 0.03000 (17) | 0.03899 (18) | -0.00180 (11) | 0.00341 (12) | 0.00317 (13) |
| Cl1 | 0.0357 (10) | 0.0525 (12) | 0.0525 (12) | 0.0011 (9) | -0.0018 (9) | 0.0159 (10) |
| Cl2 | 0.0363 (11) | 0.0537 (12) | 0.0566 (12) | -0.0171 (9) | 0.0036 (9) | 0.0119 (10) |
| Cl3 | 0.124 (5) | 0.164 (5) | 0.145 (5) | 0.039 (4) | 0.043 (4) | 0.027 (4) |
| Cl4 | 0.175 (10) | 0.188 (10) | 0.120 (6) | 0.021 (7) | -0.017 (6) | -0.015 (6) |
| Cl5 | 0.102 (4) | 0.108 (4) | 0.212 (10) | -0.007 (3) | 0.013 (5) | 0.006 (4) |

| | | | | | | |
|------|-------------|-------------|-------------|-------------|------------|-------------|
| Cl3' | 0.20 (3) | 0.20 (3) | 0.20 (3) | 0.00 (2) | 0.04 (3) | -0.01 (2) |
| Cl4' | 0.17 (3) | 0.149 (19) | 0.15 (2) | 0.022 (17) | 0.006 (18) | -0.001 (15) |
| Cl5' | 0.15 (2) | 0.17 (3) | 0.18 (3) | -0.004 (19) | 0.01 (2) | 0.00 (2) |
| P1 | 0.0273 (10) | 0.0259 (9) | 0.0416 (11) | -0.0011 (7) | 0.0046 (8) | 0.0021 (8) |
| P2 | 0.0331 (11) | 0.0335 (10) | 0.0403 (11) | -0.0019 (8) | 0.0019 (9) | 0.0046 (9) |
| C1 | 0.034 (4) | 0.039 (4) | 0.052 (5) | -0.001 (3) | 0.007 (4) | 0.003 (4) |
| C2 | 0.041 (5) | 0.059 (5) | 0.065 (6) | -0.003 (4) | 0.015 (4) | 0.000 (5) |
| C3 | 0.049 (6) | 0.088 (8) | 0.083 (7) | -0.004 (5) | 0.025 (5) | -0.008 (6) |
| C4 | 0.051 (6) | 0.080 (7) | 0.074 (7) | 0.020 (5) | 0.016 (5) | -0.003 (6) |
| C5 | 0.058 (6) | 0.057 (6) | 0.069 (6) | 0.019 (5) | 0.011 (5) | -0.006 (5) |
| C6 | 0.045 (5) | 0.048 (5) | 0.054 (5) | 0.004 (4) | 0.012 (4) | 0.004 (4) |
| C7 | 0.035 (4) | 0.037 (4) | 0.049 (5) | 0.000 (3) | 0.010 (4) | 0.009 (4) |
| C8 | 0.055 (5) | 0.047 (5) | 0.052 (5) | 0.002 (4) | 0.014 (4) | 0.009 (4) |
| C9 | 0.071 (7) | 0.069 (6) | 0.057 (6) | 0.002 (5) | 0.013 (5) | 0.014 (5) |
| C10 | 0.064 (6) | 0.057 (6) | 0.062 (6) | 0.012 (4) | 0.014 (5) | 0.027 (5) |
| C11 | 0.062 (6) | 0.047 (5) | 0.067 (6) | 0.008 (4) | 0.013 (5) | 0.013 (5) |
| C12 | 0.049 (5) | 0.040 (5) | 0.056 (5) | 0.002 (4) | 0.008 (4) | 0.005 (4) |
| C13 | 0.036 (4) | 0.033 (4) | 0.048 (5) | -0.004 (3) | 0.003 (4) | 0.002 (4) |
| C14 | 0.046 (5) | 0.052 (5) | 0.061 (5) | -0.006 (4) | 0.005 (4) | -0.001 (5) |
| C15 | 0.061 (6) | 0.063 (6) | 0.073 (7) | -0.016 (5) | -0.004 (5) | -0.007 (6) |
| C16 | 0.080 (8) | 0.056 (6) | 0.072 (7) | -0.013 (5) | 0.000 (6) | -0.013 (5) |
| C17 | 0.067 (7) | 0.056 (6) | 0.072 (6) | 0.002 (5) | 0.008 (5) | -0.014 (5) |
| C18 | 0.044 (5) | 0.048 (5) | 0.059 (6) | -0.003 (4) | 0.006 (4) | -0.004 (4) |
| C19 | 0.041 (5) | 0.043 (4) | 0.053 (5) | 0.000 (4) | -0.001 (4) | 0.011 (4) |
| C20 | 0.049 (6) | 0.054 (5) | 0.058 (6) | 0.000 (4) | 0.001 (4) | 0.007 (5) |
| C21 | 0.043 (6) | 0.069 (6) | 0.082 (7) | 0.001 (5) | -0.001 (5) | 0.010 (6) |
| C22 | 0.057 (7) | 0.080 (7) | 0.079 (8) | -0.007 (5) | -0.009 (6) | -0.003 (6) |
| C23 | 0.067 (7) | 0.072 (7) | 0.070 (7) | -0.010 (5) | -0.008 (6) | -0.007 (6) |
| C24 | 0.052 (6) | 0.058 (5) | 0.055 (6) | -0.002 (4) | 0.000 (4) | -0.002 (5) |
| C25 | 0.042 (5) | 0.037 (4) | 0.055 (5) | -0.001 (3) | 0.004 (4) | 0.004 (4) |
| C26 | 0.052 (5) | 0.043 (5) | 0.064 (6) | -0.001 (4) | 0.009 (4) | 0.004 (5) |
| C27 | 0.075 (7) | 0.059 (6) | 0.079 (7) | -0.002 (5) | 0.005 (6) | -0.009 (5) |
| C28 | 0.075 (8) | 0.053 (6) | 0.096 (9) | 0.008 (5) | 0.010 (7) | -0.001 (6) |
| C29 | 0.070 (7) | 0.059 (6) | 0.087 (8) | 0.010 (5) | 0.003 (6) | 0.012 (6) |
| C30 | 0.060 (6) | 0.046 (5) | 0.065 (6) | 0.003 (4) | 0.001 (5) | 0.007 (5) |
| C31 | 0.039 (4) | 0.044 (5) | 0.042 (5) | -0.005 (3) | 0.006 (4) | 0.005 (4) |
| C32 | 0.057 (6) | 0.049 (5) | 0.054 (5) | -0.001 (4) | 0.008 (4) | 0.011 (4) |
| C33 | 0.066 (6) | 0.060 (6) | 0.052 (5) | -0.011 (5) | 0.010 (5) | 0.019 (5) |
| C34 | 0.054 (6) | 0.077 (7) | 0.056 (6) | 0.005 (5) | 0.013 (5) | 0.012 (5) |
| C35 | 0.052 (6) | 0.064 (6) | 0.058 (6) | 0.012 (4) | 0.010 (5) | 0.004 (5) |
| C36 | 0.055 (6) | 0.054 (5) | 0.055 (6) | 0.005 (4) | 0.010 (5) | 0.014 (4) |
| C37 | 0.102 (11) | 0.098 (9) | 0.115 (11) | 0.020 (8) | 0.009 (9) | -0.023 (9) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------|-------------|---------|------------|
| Pt1—P1 | 2.2481 (17) | C15—C16 | 1.362 (12) |
| Pt1—P2 | 2.2658 (19) | C15—H15 | 0.9300 |
| Pt1—Cl1 | 2.3244 (19) | C16—C17 | 1.367 (12) |
| Pt1—Cl2 | 2.3548 (17) | C16—H16 | 0.9300 |

supplementary materials

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|-------------|------------|-------------|------------|
| Cl3—C37 | 1.758 (14) | C17—C18 | 1.373 (11) |
| Cl4—C37 | 1.697 (17) | C17—H17 | 0.9300 |
| Cl5—C37 | 1.693 (15) | C18—H18 | 0.9300 |
| Cl3'—C37 | 1.79 (3) | C19—C20 | 1.397 (11) |
| Cl4'—C37 | 1.67 (3) | C19—C24 | 1.404 (11) |
| Cl5'—C37 | 1.70 (5) | C20—C21 | 1.390 (12) |
| P1—C1 | 1.809 (7) | C20—H20 | 0.9300 |
| P1—C13 | 1.828 (8) | C21—C22 | 1.347 (14) |
| P1—C7 | 1.829 (7) | C21—H21 | 0.9300 |
| P2—C25 | 1.818 (7) | C22—C23 | 1.347 (13) |
| P2—C19 | 1.825 (8) | C22—H22 | 0.9300 |
| P2—C31 | 1.833 (7) | C23—C24 | 1.375 (12) |
| C1—C6 | 1.388 (10) | C23—H23 | 0.9300 |
| C1—C2 | 1.389 (10) | C24—H24 | 0.9300 |
| C2—C3 | 1.369 (11) | C25—C26 | 1.387 (11) |
| C2—H2 | 0.9300 | C25—C30 | 1.390 (11) |
| C3—C4 | 1.368 (12) | C26—C27 | 1.399 (11) |
| C3—H3 | 0.9300 | C26—H26 | 0.9300 |
| C4—C5 | 1.356 (12) | C27—C28 | 1.369 (14) |
| C4—H4 | 0.9300 | C27—H27 | 0.9300 |
| C5—C6 | 1.383 (10) | C28—C29 | 1.338 (14) |
| C5—H5 | 0.9300 | C28—H28 | 0.9300 |
| C6—H6 | 0.9300 | C29—C30 | 1.377 (11) |
| C7—C8 | 1.372 (10) | C29—H29 | 0.9300 |
| C7—C12 | 1.394 (10) | C30—H30 | 0.9300 |
| C8—C9 | 1.386 (11) | C31—C36 | 1.374 (10) |
| C8—H8 | 0.9300 | C31—C32 | 1.390 (10) |
| C9—C10 | 1.415 (12) | C32—C33 | 1.376 (10) |
| C9—H9 | 0.9300 | C32—H32 | 0.9300 |
| C10—C11 | 1.344 (12) | C33—C34 | 1.362 (11) |
| C10—H10 | 0.9300 | C33—H33 | 0.9300 |
| C11—C12 | 1.379 (10) | C34—C35 | 1.378 (11) |
| C11—H11 | 0.9300 | C34—H34 | 0.9300 |
| C12—H12 | 0.9300 | C35—C36 | 1.353 (12) |
| C13—C18 | 1.380 (10) | C35—H35 | 0.9300 |
| C13—C14 | 1.380 (10) | C36—H36 | 0.9300 |
| C14—C15 | 1.391 (11) | C37—H37 | 0.9800 |
| C14—H14 | 0.9300 | | |
| P1—Pt1—P2 | 97.43 (7) | C24—C19—P2 | 121.3 (6) |
| P1—Pt1—Cl1 | 89.85 (7) | C21—C20—C19 | 119.9 (9) |
| P2—Pt1—Cl1 | 172.47 (6) | C21—C20—H20 | 120.1 |
| P1—Pt1—Cl2 | 176.28 (7) | C19—C20—H20 | 120.1 |
| P2—Pt1—Cl2 | 86.26 (7) | C22—C21—C20 | 119.7 (9) |
| Cl1—Pt1—Cl2 | 86.48 (7) | C22—C21—H21 | 120.2 |
| C1—P1—C13 | 111.8 (3) | C20—C21—H21 | 120.2 |
| C1—P1—C7 | 100.3 (3) | C23—C22—C21 | 121.9 (10) |
| C13—P1—C7 | 104.3 (3) | C23—C22—H22 | 119.1 |
| C1—P1—Pt1 | 113.7 (2) | C21—C22—H22 | 119.1 |
| C13—P1—Pt1 | 110.4 (2) | C22—C23—C24 | 120.5 (10) |

| | | | |
|-------------|-----------|---------------|------------|
| C7—P1—Pt1 | 115.6 (2) | C22—C23—H23 | 119.7 |
| C25—P2—C19 | 101.0 (4) | C24—C23—H23 | 119.7 |
| C25—P2—C31 | 105.9 (3) | C23—C24—C19 | 119.6 (9) |
| C19—P2—C31 | 103.7 (4) | C23—C24—H24 | 120.2 |
| C25—P2—Pt1 | 114.3 (3) | C19—C24—H24 | 120.2 |
| C19—P2—Pt1 | 122.1 (3) | C26—C25—C30 | 118.9 (7) |
| C31—P2—Pt1 | 108.3 (3) | C26—C25—P2 | 120.2 (6) |
| C6—C1—C2 | 117.7 (7) | C30—C25—P2 | 121.0 (6) |
| C6—C1—P1 | 119.4 (5) | C25—C26—C27 | 119.8 (9) |
| C2—C1—P1 | 122.8 (6) | C25—C26—H26 | 120.1 |
| C3—C2—C1 | 120.3 (8) | C27—C26—H26 | 120.1 |
| C3—C2—H2 | 119.9 | C28—C27—C26 | 119.2 (10) |
| C1—C2—H2 | 119.9 | C28—C27—H27 | 120.4 |
| C4—C3—C2 | 120.8 (9) | C26—C27—H27 | 120.4 |
| C4—C3—H3 | 119.6 | C29—C28—C27 | 121.3 (10) |
| C2—C3—H3 | 119.6 | C29—C28—H28 | 119.4 |
| C5—C4—C3 | 120.2 (8) | C27—C28—H28 | 119.4 |
| C5—C4—H4 | 119.9 | C28—C29—C30 | 120.8 (10) |
| C3—C4—H4 | 119.9 | C28—C29—H29 | 119.6 |
| C4—C5—C6 | 119.5 (9) | C30—C29—H29 | 119.6 |
| C4—C5—H5 | 120.2 | C29—C30—C25 | 120.0 (9) |
| C6—C5—H5 | 120.2 | C29—C30—H30 | 120.0 |
| C5—C6—C1 | 121.2 (8) | C25—C30—H30 | 120.0 |
| C5—C6—H6 | 119.4 | C36—C31—C32 | 118.4 (7) |
| C1—C6—H6 | 119.4 | C36—C31—P2 | 119.6 (6) |
| C8—C7—C12 | 118.8 (7) | C32—C31—P2 | 122.0 (6) |
| C8—C7—P1 | 119.0 (6) | C33—C32—C31 | 120.1 (8) |
| C12—C7—P1 | 122.2 (6) | C33—C32—H32 | 119.9 |
| C7—C8—C9 | 121.4 (8) | C31—C32—H32 | 119.9 |
| C7—C8—H8 | 119.3 | C34—C33—C32 | 120.7 (8) |
| C9—C8—H8 | 119.3 | C34—C33—H33 | 119.6 |
| C8—C9—C10 | 118.0 (9) | C32—C33—H33 | 119.6 |
| C8—C9—H9 | 121.0 | C33—C34—C35 | 118.8 (8) |
| C10—C9—H9 | 121.0 | C33—C34—H34 | 120.6 |
| C11—C10—C9 | 120.9 (8) | C35—C34—H34 | 120.6 |
| C11—C10—H10 | 119.5 | C36—C35—C34 | 121.1 (8) |
| C9—C10—H10 | 119.5 | C36—C35—H35 | 119.4 |
| C10—C11—C12 | 120.2 (8) | C34—C35—H35 | 119.4 |
| C10—C11—H11 | 119.9 | C35—C36—C31 | 120.8 (8) |
| C12—C11—H11 | 119.9 | C35—C36—H36 | 119.6 |
| C11—C12—C7 | 120.6 (8) | C31—C36—H36 | 119.6 |
| C11—C12—H12 | 119.7 | C14'—C37—Cl5 | 51.1 (10) |
| C7—C12—H12 | 119.7 | C14'—C37—Cl4 | 134.5 (11) |
| C18—C13—C14 | 119.9 (7) | Cl5—C37—Cl4 | 114.9 (10) |
| C18—C13—P1 | 114.9 (6) | Cl4'—C37—Cl5' | 133 (2) |
| C14—C13—P1 | 125.1 (6) | Cl5—C37—Cl5' | 143.7 (16) |
| C13—C14—C15 | 118.9 (8) | Cl4—C37—Cl5' | 31.2 (11) |
| C13—C14—H14 | 120.5 | Cl4'—C37—Cl3 | 55.8 (11) |
| C15—C14—H14 | 120.5 | Cl5—C37—Cl3 | 106.5 (8) |

supplementary materials

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|----------------|-------------|-----------------|------------|
| C16—C15—C14 | 120.4 (9) | C14—C37—Cl3 | 110.0 (9) |
| C16—C15—H15 | 119.8 | Cl5'—C37—Cl3 | 86.0 (16) |
| C14—C15—H15 | 119.8 | Cl4'—C37—Cl3' | 92.8 (15) |
| C15—C16—C17 | 120.7 (9) | Cl5—C37—Cl3' | 48.8 (12) |
| C15—C16—H16 | 119.7 | Cl4—C37—Cl3' | 67.4 (13) |
| C17—C16—H16 | 119.7 | Cl5'—C37—Cl3' | 98.4 (17) |
| C16—C17—C18 | 119.6 (9) | Cl3—C37—Cl3' | 135.1 (12) |
| C16—C17—H17 | 120.2 | Cl4'—C37—H37 | 117.1 |
| C18—C17—H17 | 120.2 | Cl5—C37—H37 | 108.4 |
| C17—C18—C13 | 120.5 (8) | Cl4—C37—H37 | 108.4 |
| C17—C18—H18 | 119.8 | Cl5'—C37—H37 | 99.0 |
| C13—C18—H18 | 119.8 | Cl3—C37—H37 | 108.4 |
| C20—C19—C24 | 118.4 (8) | Cl3'—C37—H37 | 114.8 |
| C20—C19—P2 | 120.3 (7) | | |
| P2—Pt1—P1—C1 | 65.2 (3) | Pt1—P1—C13—C14 | 137.5 (6) |
| Cl1—Pt1—P1—C1 | -116.7 (3) | C18—C13—C14—C15 | 1.2 (12) |
| Cl2—Pt1—P1—C1 | -107.5 (11) | P1—C13—C14—C15 | 177.1 (6) |
| P2—Pt1—P1—C13 | -61.5 (3) | C13—C14—C15—C16 | -2.4 (13) |
| Cl1—Pt1—P1—C13 | 116.6 (3) | C14—C15—C16—C17 | 2.4 (14) |
| Cl2—Pt1—P1—C13 | 125.9 (10) | C15—C16—C17—C18 | -1.2 (14) |
| P2—Pt1—P1—C7 | -179.5 (3) | C16—C17—C18—C13 | 0.0 (13) |
| Cl1—Pt1—P1—C7 | -1.4 (3) | C14—C13—C18—C17 | 0.0 (12) |
| Cl2—Pt1—P1—C7 | 7.8 (11) | P1—C13—C18—C17 | -176.4 (6) |
| P1—Pt1—P2—C25 | -107.0 (3) | C25—P2—C19—C20 | 44.4 (7) |
| Cl1—Pt1—P2—C25 | 87.8 (6) | C31—P2—C19—C20 | 153.9 (6) |
| Cl2—Pt1—P2—C25 | 72.6 (3) | Pt1—P2—C19—C20 | -83.8 (7) |
| P1—Pt1—P2—C19 | 15.1 (3) | C25—P2—C19—C24 | -133.6 (7) |
| Cl1—Pt1—P2—C19 | -150.1 (6) | C31—P2—C19—C24 | -24.0 (7) |
| Cl2—Pt1—P2—C19 | -165.4 (3) | Pt1—P2—C19—C24 | 98.3 (7) |
| P1—Pt1—P2—C31 | 135.3 (3) | C24—C19—C20—C21 | 0.6 (12) |
| Cl1—Pt1—P2—C31 | -30.0 (6) | P2—C19—C20—C21 | -177.4 (6) |
| Cl2—Pt1—P2—C31 | -45.2 (3) | C19—C20—C21—C22 | -1.3 (13) |
| C13—P1—C1—C6 | 133.7 (6) | C20—C21—C22—C23 | 1.8 (16) |
| C7—P1—C1—C6 | -116.3 (7) | C21—C22—C23—C24 | -1.6 (17) |
| Pt1—P1—C1—C6 | 7.8 (7) | C22—C23—C24—C19 | 1.0 (14) |
| C13—P1—C1—C2 | -50.2 (8) | C20—C19—C24—C23 | -0.5 (12) |
| C7—P1—C1—C2 | 59.9 (8) | P2—C19—C24—C23 | 177.5 (7) |
| Pt1—P1—C1—C2 | -176.1 (6) | C19—P2—C25—C26 | -142.3 (6) |
| C6—C1—C2—C3 | -4.2 (13) | C31—P2—C25—C26 | 109.8 (7) |
| P1—C1—C2—C3 | 179.6 (7) | Pt1—P2—C25—C26 | -9.3 (7) |
| C1—C2—C3—C4 | 2.6 (15) | C19—P2—C25—C30 | 37.7 (7) |
| C2—C3—C4—C5 | 1.5 (16) | C31—P2—C25—C30 | -70.2 (7) |
| C3—C4—C5—C6 | -3.8 (15) | Pt1—P2—C25—C30 | 170.7 (6) |
| C4—C5—C6—C1 | 2.2 (13) | C30—C25—C26—C27 | -0.8 (12) |
| C2—C1—C6—C5 | 1.8 (12) | P2—C25—C26—C27 | 179.1 (6) |
| P1—C1—C6—C5 | 178.2 (7) | C25—C26—C27—C28 | -0.4 (14) |
| C1—P1—C7—C8 | 49.8 (7) | C26—C27—C28—C29 | 2.3 (16) |
| C13—P1—C7—C8 | 165.7 (6) | C27—C28—C29—C30 | -2.8 (17) |
| Pt1—P1—C7—C8 | -72.9 (6) | C28—C29—C30—C25 | 1.5 (15) |

| | | | |
|----------------|------------|-----------------|------------|
| C1—P1—C7—C12 | −129.5 (6) | C26—C25—C30—C29 | 0.3 (12) |
| C13—P1—C7—C12 | −13.7 (7) | P2—C25—C30—C29 | −179.6 (7) |
| Pt1—P1—C7—C12 | 107.8 (6) | C25—P2—C31—C36 | −174.3 (7) |
| C12—C7—C8—C9 | −1.1 (12) | C19—P2—C31—C36 | 79.7 (7) |
| P1—C7—C8—C9 | 179.5 (6) | Pt1—P2—C31—C36 | −51.3 (7) |
| C7—C8—C9—C10 | 1.2 (13) | C25—P2—C31—C32 | 5.0 (8) |
| C8—C9—C10—C11 | −0.8 (13) | C19—P2—C31—C32 | −100.9 (7) |
| C9—C10—C11—C12 | 0.3 (13) | Pt1—P2—C31—C32 | 128.1 (6) |
| C10—C11—C12—C7 | −0.2 (12) | C36—C31—C32—C33 | 0.9 (12) |
| C8—C7—C12—C11 | 0.6 (11) | P2—C31—C32—C33 | −178.5 (6) |
| P1—C7—C12—C11 | 180.0 (6) | C31—C32—C33—C34 | −1.4 (13) |
| C1—P1—C13—C18 | −174.0 (6) | C32—C33—C34—C35 | 0.0 (13) |
| C7—P1—C13—C18 | 78.5 (6) | C33—C34—C35—C36 | 1.9 (14) |
| Pt1—P1—C13—C18 | −46.3 (6) | C34—C35—C36—C31 | −2.4 (14) |
| C1—P1—C13—C14 | 9.9 (8) | C32—C31—C36—C35 | 1.0 (13) |
| C7—P1—C13—C14 | −97.7 (7) | P2—C31—C36—C35 | −179.7 (7) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| C3—H3···Cl1 ⁱ | 0.93 | 2.80 | 3.670 (10) | 157 |
| C37—H37···Cl2 ⁱⁱ | 0.98 | 2.43 | 3.390 (15) | 165 |

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

supplementary materials

Fig. 1

