

[1,1'-Bis(diphenylphosphino)cobalto-cenium- κ^2P,P']dichloridoplatinum(II) hexafluoridophosphate

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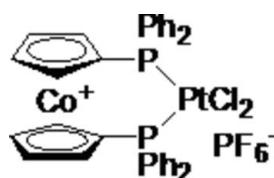
Received 22 June 2009; accepted 15 July 2009

Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$; R factor = 0.040; wR factor = 0.092; data-to-parameter ratio = 17.7.

The title bimetallic compound, $[\text{PtCl}_2\{\text{Co}(\text{C}_{17}\text{H}_{14}\text{P})_2\}]\text{PF}_6$, was obtained by reaction of 1,1'-bis(diphenylphosphino)cobalto-cenium hexafluoridophosphate with bis(acetonitrile)dichloridoplatinum. The Pt^{II} ion is four-coordinated in a slightly distorted square-planar environment by two P atoms of the 1,1'-bis(diphenylphosphino)cobalto-cenium moiety and two Cl atoms. In the crystal structure, molecules are linked by weak C—H···F and C—H···Cl hydrogen bonds.

Related literature

For background to cobalocene derivatives applied as catalysts, see: Brasse *et al.* (2000); Yu *et al.* (2007). For the structure of dichloro [1,1'-bis(diphenylphosphino)ferrocene], see: Corain *et al.* (1989). For 1,1'-bis(diphenylphosphino)cobalto-cenium tetrafluoridoborate, see: Hou *et al.* (2007).



Experimental

Crystal data

| | |
|---|--------------------------------|
| $[\text{CoPt}(\text{C}_{17}\text{H}_{14}\text{P})_2\text{Cl}_2]\text{PF}_6$ | $c = 19.7670 (1)\text{ \AA}$ |
| $M_r = 968.39$ | $\alpha = 94.9780 (1)^\circ$ |
| Triclinic, $P\bar{1}$ | $\beta = 102.4230 (1)^\circ$ |
| $a = 8.9730 (1)\text{ \AA}$ | $\gamma = 114.2320 (1)^\circ$ |
| $b = 10.8770 (1)\text{ \AA}$ | $V = 1684.54 (3)\text{ \AA}^3$ |

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 5.00\text{ mm}^{-1}$
 $T = 293\text{ K}$
 $0.20 \times 0.10 \times 0.10\text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
 $T_{\min} = 0.435$, $T_{\max} = 0.635$
17964 measured reflections
7506 independent reflections
6245 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.080$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.092$
 $S = 1.00$
424 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.98\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.19\text{ e \AA}^{-3}$
7506 reflections

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|------------------------------|--------------|--------------------|-------------|----------------------|
| C3—H3···F2 ⁱ | 0.98 | 2.32 | 3.190 (11) | 148 |
| C4—H4···Cl1 ⁱⁱ | 0.98 | 2.80 | 3.448 (7) | 124 |
| C7—H7···F5 | 0.98 | 2.55 | 3.513 (14) | 168 |
| C12—H12···F6 ⁱⁱⁱ | 0.93 | 2.54 | 3.267 (11) | 135 |
| C14—H14···Cl2 ⁱⁱⁱ | 0.93 | 2.79 | 3.497 (8) | 134 |
| C16—H16···Cl1 | 0.93 | 2.80 | 3.454 (7) | 128 |
| C22—H22···F5 | 0.93 | 2.51 | 3.311 (11) | 145 |

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

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 acknowledge financial support from the National Natural Science Foundation of China (No. 20572029), the New Century Excellent Talents in Universities (NCET-04-0743) and the Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (No. 705039).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2085).

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supplementary materials

Acta Cryst. (2009). E65, m960 [doi:10.1107/S1600536809027925]

[1,1'-Bis(diphenylphosphino)cobaltocenium- κ^2P,P']dichloridoplatinum(II) hexafluoridophosphate

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Comment

Cobaltocene derivatives have been applied as catalysts in cross-coupling reactions (Brasse *et al.*, 2000). As part of our investigations of new catalysts, we have focused our attention on cobaltocenium compounds. Some complexes, such as 1,1'-bis(diphenylphosphino)cobaltocenium tetrafluoridoborate, have been obtained and reported (Hou *et al.*, 2007). Herein, we report the structure of the title compound, (I) (Fig. 1), which is very similar to the complex dichloro [1,1'-bis(diphenylphosphino)ferrocene] (Corain *et al.*, 1989). The Pt I^+ metal ion is in an essentially square-planar environment defined by the two Cl atoms and the two P atoms. The angle between the plane P—Pt—P and the plane Cl—Pt—Cl is 4.0 (3) $^\circ$. The bond angle of the two P atoms at the Pt atom is 100.64 (5) $^\circ$, with the two Cl atoms it is 86.08 (5) $^\circ$. The two substituted Cp rings are staggered and are essentially parallel with an interplanar angle of 3.62 (2) $^\circ$. The crystal structure contains non-bonded C—H···F and C—H···Cl interactions (Fig. 2).

Experimental

A mixture of 1,1'-bis(diphenylphosphino)cobaltocenium hexafluoridophosphate (70.2 mg, 0.1 mmol) and bis(acetonitrile)dichloroplatinum (34.8 mg, 0.1 mmol) in CH₂Cl₂ (10 ml) was stirred for 4 h. The precipitate formed was separated by filtration and washed with Et₂O and water, and dried under vacuum to give an yellow powder (85.2 mg). Crystals appropriate for data collection were obtained by slow evaporation from a CH₃NO₂ solution at 293 K.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å; with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

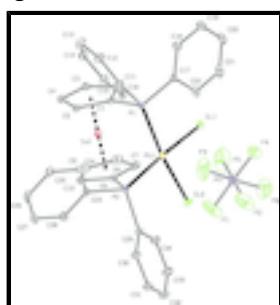


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms are omitted for clarity.

supplementary materials

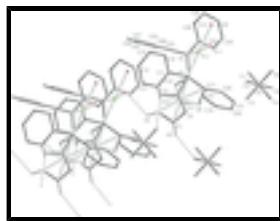


Fig. 2. Hydrogen bonding interactions in (I). H atoms not involved in hydrogen bonding have been omitted.

[1,1'-Bis(diphenylphosphino)cobaltocenium- κ^2P,P']dichloridoplatinum(II) hexafluoridophosphate

Crystal data

| | |
|-----------------------------------|---|
| $[CoPt(C_{17}H_{14}P)_2Cl_2]PF_6$ | $Z = 2$ |
| $M_r = 968.39$ | $F_{000} = 940$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.909 \text{ Mg m}^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 8.9730 (1) \text{ \AA}$ | Cell parameters from 7129 reflections |
| $b = 10.8770 (1) \text{ \AA}$ | $\theta = 2.5\text{--}27.4^\circ$ |
| $c = 19.7670 (1) \text{ \AA}$ | $\mu = 5.00 \text{ mm}^{-1}$ |
| $\alpha = 94.9780 (1)^\circ$ | $T = 293 \text{ K}$ |
| $\beta = 102.4230 (1)^\circ$ | Block, yellow |
| $\gamma = 114.2320 (1)^\circ$ | $0.20 \times 0.10 \times 0.10 \text{ mm}$ |
| $V = 1684.54 (3) \text{ \AA}^3$ | |

Data collection

| | |
|---|--|
| Bruker SMART CCD area-detector diffractometer | 7506 independent reflections |
| Radiation source: fine-focus sealed tube | 6245 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.080$ |
| $T = 293 \text{ K}$ | $\theta_{\max} = 27.5^\circ$ |
| φ and ω scans | $\theta_{\min} = 1.1^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2004) | $h = -11 \rightarrow 11$ |
| $T_{\min} = 0.435$, $T_{\max} = 0.635$ | $k = -13 \rightarrow 13$ |
| 17964 measured reflections | $l = -25 \rightarrow 25$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | H-atom parameters constrained |
| $wR(F^2) = 0.092$ | $w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.1224P]$ |
| $S = 1.00$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 7506 reflections | $(\Delta/\sigma)_{\max} = 0.027$ |
| | $\Delta\rho_{\max} = 1.98 \text{ e \AA}^{-3}$ |

424 parameters $\Delta\rho_{\min} = -1.19 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct Extinction correction: none
 methods

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|---------------|---------------|----------------------------------|
| Pt1 | 0.39843 (2) | 0.173677 (19) | 0.691223 (10) | 0.02720 (8) |
| C1 | 0.1265 (6) | 0.0476 (5) | 0.8029 (3) | 0.0310 (11) |
| C2 | 0.1575 (7) | 0.0917 (6) | 0.8766 (3) | 0.0393 (13) |
| H2 | 0.2662 | 0.1217 | 0.9124 | 0.047* |
| C3 | 0.0069 (7) | 0.0887 (6) | 0.8896 (3) | 0.0402 (14) |
| H3 | -0.0069 | 0.1162 | 0.9355 | 0.048* |
| C4 | -0.1191 (7) | 0.0395 (6) | 0.8243 (3) | 0.0385 (13) |
| H4 | -0.2358 | 0.0284 | 0.8171 | 0.046* |
| C5 | -0.0475 (6) | 0.0153 (5) | 0.7704 (3) | 0.0335 (12) |
| H5 | -0.1066 | -0.0182 | 0.7199 | 0.040* |
| C6 | 0.1783 (7) | 0.3358 (5) | 0.7545 (3) | 0.0313 (11) |
| C7 | 0.2929 (8) | 0.3902 (6) | 0.8247 (3) | 0.0453 (15) |
| H7 | 0.4113 | 0.4042 | 0.8385 | 0.054* |
| C8 | 0.2032 (11) | 0.4171 (7) | 0.8706 (4) | 0.061 (2) |
| H8 | 0.2486 | 0.4506 | 0.9218 | 0.074* |
| C9 | 0.0375 (11) | 0.3835 (7) | 0.8310 (4) | 0.060 (2) |
| H9 | -0.0523 | 0.3899 | 0.8496 | 0.072* |
| C10 | 0.0197 (8) | 0.3319 (6) | 0.7586 (3) | 0.0462 (15) |
| H10 | -0.0830 | 0.3002 | 0.7191 | 0.055* |
| C11 | 0.1492 (7) | -0.1487 (5) | 0.7122 (3) | 0.0350 (12) |
| C12 | 0.0321 (8) | -0.2418 (6) | 0.7413 (3) | 0.0507 (16) |
| H12 | 0.0269 | -0.2148 | 0.7864 | 0.061* |
| C13 | -0.0751 (8) | -0.3725 (7) | 0.7043 (4) | 0.0605 (19) |
| H13 | -0.1526 | -0.4341 | 0.7241 | 0.073* |
| C14 | -0.0672 (8) | -0.4123 (6) | 0.6369 (4) | 0.0574 (18) |
| H14 | -0.1420 | -0.5001 | 0.6109 | 0.069* |
| C15 | 0.0499 (8) | -0.3231 (7) | 0.6084 (4) | 0.0519 (16) |
| H15 | 0.0562 | -0.3515 | 0.5638 | 0.062* |
| C16 | 0.1584 (7) | -0.1917 (6) | 0.6453 (3) | 0.0409 (14) |
| H16 | 0.2376 | -0.1316 | 0.6257 | 0.049* |

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| | | | | |
|-----|--------------|--------------|--------------|--------------|
| C17 | 0.4359 (7) | 0.0302 (6) | 0.8356 (3) | 0.0373 (13) |
| C18 | 0.4344 (8) | -0.0865 (7) | 0.8568 (3) | 0.0513 (16) |
| H18 | 0.3546 | -0.1725 | 0.8305 | 0.062* |
| C19 | 0.5543 (11) | -0.0755 (10) | 0.9187 (4) | 0.073 (2) |
| H19 | 0.5538 | -0.1545 | 0.9335 | 0.088* |
| C20 | 0.6699 (10) | 0.0491 (11) | 0.9567 (4) | 0.074 (3) |
| H20 | 0.7482 | 0.0555 | 0.9978 | 0.089* |
| C21 | 0.6736 (8) | 0.1670 (10) | 0.9353 (4) | 0.068 (2) |
| H21 | 0.7538 | 0.2524 | 0.9622 | 0.081* |
| C22 | 0.5600 (7) | 0.1594 (7) | 0.8746 (3) | 0.0495 (16) |
| H22 | 0.5650 | 0.2392 | 0.8594 | 0.059* |
| C23 | 0.0296 (6) | 0.1815 (5) | 0.6113 (3) | 0.0295 (11) |
| C24 | -0.0224 (7) | 0.0419 (6) | 0.5888 (3) | 0.0367 (13) |
| H24 | 0.0462 | 0.0008 | 0.6067 | 0.044* |
| C25 | -0.1782 (7) | -0.0353 (6) | 0.5390 (3) | 0.0433 (14) |
| H25 | -0.2142 | -0.1290 | 0.5245 | 0.052* |
| C26 | -0.2803 (7) | 0.0236 (7) | 0.5108 (3) | 0.0494 (17) |
| H26 | -0.3833 | -0.0292 | 0.4769 | 0.059* |
| C27 | -0.2286 (8) | 0.1602 (7) | 0.5332 (3) | 0.0497 (16) |
| H27 | -0.2978 | 0.2006 | 0.5146 | 0.060* |
| C28 | -0.0737 (7) | 0.2407 (6) | 0.5835 (3) | 0.0419 (14) |
| H28 | -0.0399 | 0.3340 | 0.5982 | 0.050* |
| C29 | 0.3237 (7) | 0.4478 (6) | 0.6492 (3) | 0.0360 (12) |
| C30 | 0.3094 (8) | 0.4536 (6) | 0.5787 (3) | 0.0458 (15) |
| H30 | 0.2458 | 0.3736 | 0.5445 | 0.055* |
| C31 | 0.3895 (9) | 0.5784 (8) | 0.5587 (4) | 0.0591 (19) |
| H31 | 0.3807 | 0.5818 | 0.5112 | 0.071* |
| C32 | 0.4826 (9) | 0.6979 (7) | 0.6099 (4) | 0.063 (2) |
| H32 | 0.5356 | 0.7819 | 0.5967 | 0.075* |
| C33 | 0.4963 (9) | 0.6918 (7) | 0.6794 (4) | 0.0629 (19) |
| H33 | 0.5592 | 0.7720 | 0.7136 | 0.075* |
| C34 | 0.4184 (8) | 0.5689 (6) | 0.6996 (3) | 0.0513 (16) |
| H34 | 0.4289 | 0.5664 | 0.7472 | 0.062* |
| Cl1 | 0.57300 (18) | 0.06097 (16) | 0.69406 (8) | 0.0458 (4) |
| Cl2 | 0.5467 (2) | 0.30193 (16) | 0.61893 (9) | 0.0502 (4) |
| Co1 | 0.08481 (9) | 0.21409 (8) | 0.82014 (4) | 0.03369 (17) |
| P1 | 0.27781 (16) | 0.02746 (14) | 0.75901 (7) | 0.0295 (3) |
| P2 | 0.23250 (16) | 0.28380 (13) | 0.67663 (7) | 0.0285 (3) |
| F1 | 0.7096 (13) | 0.6711 (9) | 0.8492 (4) | 0.209 (4) |
| F4 | 0.9060 (8) | 0.6276 (8) | 0.9842 (3) | 0.129 (2) |
| F3 | 0.6545 (11) | 0.6101 (15) | 0.9389 (5) | 0.255 (6) |
| F5 | 0.7334 (12) | 0.4950 (8) | 0.8797 (7) | 0.265 (6) |
| F2 | 0.8821 (13) | 0.7923 (8) | 0.9449 (5) | 0.230 (5) |
| F6 | 0.9614 (11) | 0.6650 (12) | 0.8885 (4) | 0.211 (5) |
| P3 | 0.8058 (3) | 0.6409 (2) | 0.91318 (10) | 0.0653 (5) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|-------------|-------------|-------------|
| Pt1 | 0.02182 (10) | 0.02686 (12) | 0.03064 (12) | 0.00777 (8) | 0.00884 (8) | 0.00572 (8) |
| C1 | 0.030 (3) | 0.028 (3) | 0.037 (3) | 0.012 (2) | 0.013 (2) | 0.012 (2) |
| C2 | 0.036 (3) | 0.054 (4) | 0.029 (3) | 0.019 (3) | 0.010 (2) | 0.012 (3) |
| C3 | 0.045 (3) | 0.048 (4) | 0.036 (3) | 0.022 (3) | 0.021 (3) | 0.018 (3) |
| C4 | 0.032 (3) | 0.041 (3) | 0.046 (3) | 0.014 (2) | 0.017 (3) | 0.014 (3) |
| C5 | 0.033 (3) | 0.032 (3) | 0.032 (3) | 0.010 (2) | 0.010 (2) | 0.005 (2) |
| C6 | 0.037 (3) | 0.024 (3) | 0.035 (3) | 0.012 (2) | 0.014 (2) | 0.008 (2) |
| C7 | 0.046 (3) | 0.031 (3) | 0.038 (3) | 0.001 (3) | 0.008 (3) | -0.002 (3) |
| C8 | 0.094 (6) | 0.037 (4) | 0.043 (4) | 0.016 (4) | 0.028 (4) | 0.000 (3) |
| C9 | 0.089 (6) | 0.057 (5) | 0.067 (5) | 0.047 (4) | 0.049 (4) | 0.020 (4) |
| C10 | 0.052 (4) | 0.044 (4) | 0.059 (4) | 0.029 (3) | 0.026 (3) | 0.024 (3) |
| C11 | 0.035 (3) | 0.030 (3) | 0.043 (3) | 0.016 (2) | 0.015 (2) | 0.007 (2) |
| C12 | 0.060 (4) | 0.032 (3) | 0.059 (4) | 0.014 (3) | 0.030 (3) | 0.008 (3) |
| C13 | 0.056 (4) | 0.042 (4) | 0.081 (5) | 0.012 (3) | 0.036 (4) | 0.010 (4) |
| C14 | 0.045 (4) | 0.029 (3) | 0.085 (5) | 0.008 (3) | 0.015 (4) | -0.003 (3) |
| C15 | 0.049 (4) | 0.046 (4) | 0.055 (4) | 0.017 (3) | 0.017 (3) | -0.003 (3) |
| C16 | 0.034 (3) | 0.038 (3) | 0.048 (3) | 0.012 (3) | 0.014 (3) | 0.006 (3) |
| C17 | 0.033 (3) | 0.055 (4) | 0.036 (3) | 0.026 (3) | 0.013 (2) | 0.018 (3) |
| C18 | 0.055 (4) | 0.060 (4) | 0.057 (4) | 0.036 (3) | 0.023 (3) | 0.027 (3) |
| C19 | 0.074 (5) | 0.115 (8) | 0.068 (5) | 0.064 (5) | 0.032 (4) | 0.059 (5) |
| C20 | 0.052 (4) | 0.142 (9) | 0.049 (4) | 0.057 (5) | 0.018 (4) | 0.042 (5) |
| C21 | 0.038 (4) | 0.111 (7) | 0.043 (4) | 0.029 (4) | 0.003 (3) | 0.005 (4) |
| C22 | 0.041 (3) | 0.061 (4) | 0.047 (4) | 0.026 (3) | 0.009 (3) | 0.005 (3) |
| C23 | 0.029 (3) | 0.032 (3) | 0.028 (3) | 0.014 (2) | 0.007 (2) | 0.007 (2) |
| C24 | 0.034 (3) | 0.038 (3) | 0.039 (3) | 0.016 (2) | 0.011 (2) | 0.008 (2) |
| C25 | 0.039 (3) | 0.035 (3) | 0.042 (3) | 0.006 (3) | 0.009 (3) | -0.006 (3) |
| C26 | 0.028 (3) | 0.067 (5) | 0.040 (3) | 0.011 (3) | 0.006 (3) | -0.003 (3) |
| C27 | 0.037 (3) | 0.067 (5) | 0.052 (4) | 0.033 (3) | 0.006 (3) | 0.012 (3) |
| C28 | 0.038 (3) | 0.040 (3) | 0.049 (4) | 0.023 (3) | 0.007 (3) | 0.002 (3) |
| C29 | 0.034 (3) | 0.032 (3) | 0.041 (3) | 0.013 (2) | 0.012 (2) | 0.012 (2) |
| C30 | 0.051 (4) | 0.042 (4) | 0.048 (4) | 0.020 (3) | 0.019 (3) | 0.015 (3) |
| C31 | 0.066 (4) | 0.065 (5) | 0.060 (4) | 0.032 (4) | 0.028 (4) | 0.034 (4) |
| C32 | 0.058 (4) | 0.041 (4) | 0.092 (6) | 0.017 (3) | 0.029 (4) | 0.036 (4) |
| C33 | 0.065 (5) | 0.034 (4) | 0.070 (5) | 0.006 (3) | 0.012 (4) | 0.010 (3) |
| C34 | 0.051 (4) | 0.037 (4) | 0.050 (4) | 0.007 (3) | 0.008 (3) | 0.013 (3) |
| Cl1 | 0.0384 (7) | 0.0527 (9) | 0.0572 (9) | 0.0263 (7) | 0.0193 (7) | 0.0171 (7) |
| Cl2 | 0.0529 (9) | 0.0433 (9) | 0.0666 (10) | 0.0201 (7) | 0.0379 (8) | 0.0221 (7) |
| Co1 | 0.0351 (4) | 0.0350 (4) | 0.0317 (4) | 0.0140 (3) | 0.0140 (3) | 0.0054 (3) |
| P1 | 0.0275 (6) | 0.0304 (7) | 0.0321 (7) | 0.0127 (6) | 0.0101 (6) | 0.0091 (6) |
| P2 | 0.0282 (6) | 0.0246 (7) | 0.0307 (7) | 0.0088 (5) | 0.0100 (6) | 0.0055 (5) |
| F1 | 0.269 (10) | 0.196 (9) | 0.115 (5) | 0.133 (8) | -0.088 (6) | -0.008 (5) |
| F4 | 0.119 (5) | 0.172 (6) | 0.091 (4) | 0.062 (4) | 0.013 (3) | 0.053 (4) |
| F3 | 0.122 (6) | 0.457 (19) | 0.210 (9) | 0.118 (9) | 0.102 (7) | 0.085 (10) |
| F5 | 0.172 (8) | 0.088 (6) | 0.445 (17) | 0.039 (5) | -0.002 (10) | -0.082 (8) |

supplementary materials

| | | | | | | |
|----|-------------|-------------|-------------|-------------|------------|-------------|
| F2 | 0.255 (11) | 0.105 (6) | 0.217 (9) | 0.073 (6) | -0.119 (8) | -0.031 (6) |
| F6 | 0.165 (7) | 0.350 (15) | 0.138 (6) | 0.101 (8) | 0.091 (6) | 0.074 (8) |
| P3 | 0.0571 (11) | 0.0653 (14) | 0.0542 (11) | 0.0153 (10) | 0.0056 (9) | 0.0014 (10) |

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

| | | | |
|---------|-------------|---------|------------|
| Pt1—P2 | 2.2525 (14) | C15—H15 | 0.9300 |
| Pt1—P1 | 2.2533 (13) | C16—H16 | 0.9300 |
| Pt1—Cl2 | 2.3235 (13) | C17—C18 | 1.366 (8) |
| Pt1—Cl1 | 2.3473 (15) | C17—C22 | 1.403 (8) |
| C1—C2 | 1.424 (7) | C17—P1 | 1.828 (5) |
| C1—C5 | 1.432 (7) | C18—C19 | 1.403 (9) |
| C1—P1 | 1.833 (5) | C18—H18 | 0.9300 |
| C1—Co1 | 2.010 (5) | C19—C20 | 1.346 (12) |
| C2—C3 | 1.416 (8) | C19—H19 | 0.9300 |
| C2—Co1 | 2.025 (6) | C20—C21 | 1.374 (11) |
| C2—H2 | 0.9800 | C20—H20 | 0.9300 |
| C3—C4 | 1.409 (8) | C21—C22 | 1.367 (9) |
| C3—Co1 | 2.046 (5) | C21—H21 | 0.9300 |
| C3—H3 | 0.9800 | C22—H22 | 0.9300 |
| C4—C5 | 1.415 (7) | C23—C28 | 1.381 (8) |
| C4—Co1 | 2.049 (5) | C23—C24 | 1.390 (8) |
| C4—H4 | 0.9800 | C23—P2 | 1.816 (5) |
| C5—Co1 | 2.018 (5) | C24—C25 | 1.388 (8) |
| C5—H5 | 0.9800 | C24—H24 | 0.9300 |
| C6—C10 | 1.426 (8) | C25—C26 | 1.373 (9) |
| C6—C7 | 1.441 (8) | C25—H25 | 0.9300 |
| C6—P2 | 1.823 (5) | C26—C27 | 1.361 (9) |
| C6—Co1 | 1.999 (5) | C26—H26 | 0.9300 |
| C7—C8 | 1.420 (9) | C27—C28 | 1.394 (8) |
| C7—Co1 | 2.032 (5) | C27—H27 | 0.9300 |
| C7—H7 | 0.9800 | C28—H28 | 0.9300 |
| C8—C9 | 1.400 (10) | C29—C30 | 1.381 (8) |
| C8—Co1 | 2.058 (6) | C29—C34 | 1.391 (8) |
| C8—H8 | 0.9800 | C29—P2 | 1.818 (5) |
| C9—C10 | 1.441 (9) | C30—C31 | 1.390 (9) |
| C9—Co1 | 2.057 (7) | C30—H30 | 0.9300 |
| C9—H9 | 0.9800 | C31—C32 | 1.389 (10) |
| C10—Co1 | 2.011 (6) | C31—H31 | 0.9300 |
| C10—H10 | 0.9800 | C32—C33 | 1.364 (9) |
| C11—C16 | 1.394 (7) | C32—H32 | 0.9300 |
| C11—C12 | 1.396 (7) | C33—C34 | 1.372 (8) |
| C11—P1 | 1.810 (6) | C33—H33 | 0.9300 |
| C12—C13 | 1.369 (9) | C34—H34 | 0.9300 |
| C12—H12 | 0.9300 | F1—P3 | 1.512 (7) |
| C13—C14 | 1.392 (9) | F4—P3 | 1.550 (6) |
| C13—H13 | 0.9300 | F3—P3 | 1.472 (7) |
| C14—C15 | 1.369 (9) | F5—P3 | 1.472 (8) |
| C14—H14 | 0.9300 | F2—P3 | 1.511 (8) |

| | | | |
|-------------|------------|-------------|-----------|
| C15—C16 | 1.377 (8) | F6—P3 | 1.507 (7) |
| P2—Pt1—P1 | 100.63 (5) | C25—C24—C23 | 119.1 (5) |
| P2—Pt1—Cl2 | 88.81 (5) | C25—C24—H24 | 120.5 |
| P1—Pt1—Cl2 | 170.32 (5) | C23—C24—H24 | 120.5 |
| P2—Pt1—Cl1 | 173.88 (5) | C26—C25—C24 | 121.5 (6) |
| P1—Pt1—Cl1 | 84.37 (5) | C26—C25—H25 | 119.3 |
| Cl2—Pt1—Cl1 | 86.08 (5) | C24—C25—H25 | 119.3 |
| C2—C1—C5 | 106.8 (4) | C27—C26—C25 | 119.1 (6) |
| C2—C1—P1 | 126.3 (4) | C27—C26—H26 | 120.5 |
| C5—C1—P1 | 126.8 (4) | C25—C26—H26 | 120.5 |
| C2—C1—Co1 | 69.9 (3) | C26—C27—C28 | 121.0 (6) |
| C5—C1—Co1 | 69.5 (3) | C26—C27—H27 | 119.5 |
| P1—C1—Co1 | 128.0 (3) | C28—C27—H27 | 119.5 |
| C3—C2—C1 | 108.9 (5) | C23—C28—C27 | 119.8 (6) |
| C3—C2—Co1 | 70.4 (3) | C23—C28—H28 | 120.1 |
| C1—C2—Co1 | 68.8 (3) | C27—C28—H28 | 120.1 |
| C3—C2—H2 | 125.5 | C30—C29—C34 | 118.9 (5) |
| C1—C2—H2 | 125.5 | C30—C29—P2 | 120.7 (4) |
| Co1—C2—H2 | 125.5 | C34—C29—P2 | 120.2 (4) |
| C4—C3—C2 | 107.5 (5) | C29—C30—C31 | 120.3 (6) |
| C4—C3—Co1 | 70.0 (3) | C29—C30—H30 | 119.8 |
| C2—C3—Co1 | 68.9 (3) | C31—C30—H30 | 119.8 |
| C4—C3—H3 | 126.3 | C32—C31—C30 | 119.7 (6) |
| C2—C3—H3 | 126.3 | C32—C31—H31 | 120.2 |
| Co1—C3—H3 | 126.3 | C30—C31—H31 | 120.2 |
| C3—C4—C5 | 109.0 (5) | C33—C32—C31 | 119.8 (6) |
| C3—C4—Co1 | 69.7 (3) | C33—C32—H32 | 120.1 |
| C5—C4—Co1 | 68.5 (3) | C31—C32—H32 | 120.1 |
| C3—C4—H4 | 125.5 | C32—C33—C34 | 120.8 (7) |
| C5—C4—H4 | 125.5 | C32—C33—H33 | 119.6 |
| Co1—C4—H4 | 125.5 | C34—C33—H33 | 119.6 |
| C4—C5—C1 | 107.8 (5) | C33—C34—C29 | 120.4 (6) |
| C4—C5—Co1 | 70.8 (3) | C33—C34—H34 | 119.8 |
| C1—C5—Co1 | 68.9 (3) | C29—C34—H34 | 119.8 |
| C4—C5—H5 | 126.1 | C6—Co1—C1 | 107.7 (2) |
| C1—C5—H5 | 126.1 | C6—Co1—C10 | 41.7 (2) |
| Co1—C5—H5 | 126.1 | C1—Co1—C10 | 134.9 (2) |
| C10—C6—C7 | 107.2 (5) | C6—Co1—C5 | 111.5 (2) |
| C10—C6—P2 | 127.8 (4) | C1—Co1—C5 | 41.7 (2) |
| C7—C6—P2 | 125.0 (4) | C10—Co1—C5 | 109.1 (2) |
| C10—C6—Co1 | 69.6 (3) | C6—Co1—C2 | 134.9 (2) |
| C7—C6—Co1 | 70.3 (3) | C1—Co1—C2 | 41.3 (2) |
| P2—C6—Co1 | 125.5 (3) | C10—Co1—C2 | 175.8 (2) |
| C8—C7—C6 | 108.0 (6) | C5—Co1—C2 | 69.1 (2) |
| C8—C7—Co1 | 70.7 (4) | C6—Co1—C7 | 41.9 (2) |
| C6—C7—Co1 | 67.8 (3) | C1—Co1—C7 | 111.7 (2) |
| C8—C7—H7 | 126.0 | C10—Co1—C7 | 69.6 (3) |
| C6—C7—H7 | 126.0 | C5—Co1—C7 | 142.6 (2) |
| Co1—C7—H7 | 126.0 | C2—Co1—C7 | 109.3 (3) |

supplementary materials

| | | | |
|-------------|-----------|------------|-------------|
| C9—C8—C7 | 108.8 (6) | C6—Co1—C3 | 175.5 (2) |
| C9—C8—Co1 | 70.1 (4) | C1—Co1—C3 | 69.5 (2) |
| C7—C8—Co1 | 68.7 (3) | C10—Co1—C3 | 142.8 (2) |
| C9—C8—H8 | 125.6 | C5—Co1—C3 | 68.9 (2) |
| C7—C8—H8 | 125.6 | C2—Co1—C3 | 40.7 (2) |
| Co1—C8—H8 | 125.6 | C7—Co1—C3 | 135.3 (2) |
| C8—C9—C10 | 108.2 (6) | C6—Co1—C4 | 142.7 (2) |
| C8—C9—Co1 | 70.1 (4) | C1—Co1—C4 | 69.0 (2) |
| C10—C9—Co1 | 67.5 (3) | C10—Co1—C4 | 113.4 (2) |
| C8—C9—H9 | 125.9 | C5—Co1—C4 | 40.7 (2) |
| C10—C9—H9 | 125.9 | C2—Co1—C4 | 68.0 (2) |
| Co1—C9—H9 | 125.9 | C7—Co1—C4 | 175.4 (2) |
| C6—C10—C9 | 107.8 (6) | C3—Co1—C4 | 40.2 (2) |
| C6—C10—Co1 | 68.7 (3) | C6—Co1—C9 | 69.7 (2) |
| C9—C10—Co1 | 71.0 (4) | C1—Co1—C9 | 176.4 (2) |
| C6—C10—H10 | 126.1 | C10—Co1—C9 | 41.5 (3) |
| C9—C10—H10 | 126.1 | C5—Co1—C9 | 136.4 (3) |
| Co1—C10—H10 | 126.1 | C2—Co1—C9 | 142.3 (3) |
| C16—C11—C12 | 119.0 (5) | C7—Co1—C9 | 68.2 (3) |
| C16—C11—P1 | 120.9 (4) | C3—Co1—C9 | 113.3 (2) |
| C12—C11—P1 | 120.0 (4) | C4—Co1—C9 | 111.4 (3) |
| C13—C12—C11 | 120.8 (6) | C6—Co1—C8 | 69.6 (2) |
| C13—C12—H12 | 119.6 | C1—Co1—C8 | 142.3 (3) |
| C11—C12—H12 | 119.6 | C10—Co1—C8 | 68.9 (3) |
| C12—C13—C14 | 119.4 (6) | C5—Co1—C8 | 175.9 (3) |
| C12—C13—H13 | 120.3 | C2—Co1—C8 | 113.2 (3) |
| C14—C13—H13 | 120.3 | C7—Co1—C8 | 40.6 (2) |
| C15—C14—C13 | 120.4 (6) | C3—Co1—C8 | 110.4 (2) |
| C15—C14—H14 | 119.8 | C4—Co1—C8 | 136.2 (2) |
| C13—C14—H14 | 119.8 | C9—Co1—C8 | 39.8 (3) |
| C14—C15—C16 | 120.5 (6) | C11—P1—C17 | 108.6 (3) |
| C14—C15—H15 | 119.8 | C11—P1—C1 | 98.9 (2) |
| C16—C15—H15 | 119.8 | C17—P1—C1 | 99.8 (2) |
| C15—C16—C11 | 119.9 (5) | C11—P1—Pt1 | 114.09 (18) |
| C15—C16—H16 | 120.0 | C17—P1—Pt1 | 111.89 (17) |
| C11—C16—H16 | 120.0 | C1—P1—Pt1 | 121.89 (17) |
| C18—C17—C22 | 119.8 (6) | C23—P2—C29 | 105.9 (2) |
| C18—C17—P1 | 123.0 (5) | C23—P2—C6 | 104.9 (2) |
| C22—C17—P1 | 117.2 (5) | C29—P2—C6 | 100.4 (2) |
| C17—C18—C19 | 119.5 (7) | C23—P2—Pt1 | 112.19 (18) |
| C17—C18—H18 | 120.2 | C29—P2—Pt1 | 115.15 (18) |
| C19—C18—H18 | 120.2 | C6—P2—Pt1 | 116.92 (18) |
| C20—C19—C18 | 120.1 (8) | F5—P3—F3 | 89.2 (7) |
| C20—C19—H19 | 119.9 | F5—P3—F6 | 88.5 (6) |
| C18—C19—H19 | 119.9 | F3—P3—F6 | 176.5 (7) |
| C19—C20—C21 | 120.8 (7) | F5—P3—F2 | 177.7 (7) |
| C19—C20—H20 | 119.6 | F3—P3—F2 | 92.5 (7) |
| C21—C20—H20 | 119.6 | F6—P3—F2 | 89.9 (6) |
| C22—C21—C20 | 120.4 (8) | F5—P3—F1 | 91.4 (6) |

| | | | |
|-----------------|------------|---------------|------------|
| C22—C21—H21 | 119.8 | F3—P3—F1 | 86.0 (6) |
| C20—C21—H21 | 119.8 | F6—P3—F1 | 96.7 (6) |
| C21—C22—C17 | 119.4 (7) | F2—P3—F1 | 87.1 (5) |
| C21—C22—H22 | 120.3 | F5—P3—F4 | 95.7 (6) |
| C17—C22—H22 | 120.3 | F3—P3—F4 | 91.4 (5) |
| C28—C23—C24 | 119.5 (5) | F6—P3—F4 | 86.2 (4) |
| C28—C23—P2 | 120.8 (4) | F2—P3—F4 | 85.9 (4) |
| C24—C23—P2 | 119.7 (4) | F1—P3—F4 | 172.4 (5) |
| C5—C1—C2—C3 | -0.8 (6) | C3—C2—Co1—C1 | -120.5 (5) |
| P1—C1—C2—C3 | -177.8 (4) | C3—C2—Co1—C10 | -147 (3) |
| Co1—C1—C2—C3 | 59.1 (4) | C1—C2—Co1—C10 | -27 (4) |
| C5—C1—C2—Co1 | -59.9 (3) | C3—C2—Co1—C5 | -81.5 (4) |
| P1—C1—C2—Co1 | 123.0 (4) | C1—C2—Co1—C5 | 39.0 (3) |
| C1—C2—C3—C4 | 1.5 (7) | C3—C2—Co1—C7 | 138.4 (4) |
| Co1—C2—C3—C4 | 59.6 (4) | C1—C2—Co1—C7 | -101.2 (3) |
| C1—C2—C3—Co1 | -58.1 (4) | C1—C2—Co1—C3 | 120.5 (5) |
| C2—C3—C4—C5 | -1.6 (7) | C3—C2—Co1—C4 | -37.6 (3) |
| Co1—C3—C4—C5 | 57.3 (4) | C1—C2—Co1—C4 | 82.9 (3) |
| C2—C3—C4—Co1 | -58.9 (4) | C3—C2—Co1—C9 | 59.3 (6) |
| C3—C4—C5—C1 | 1.1 (6) | C1—C2—Co1—C9 | 179.7 (4) |
| Co1—C4—C5—C1 | 59.2 (3) | C3—C2—Co1—C8 | 94.8 (4) |
| C3—C4—C5—Co1 | -58.1 (4) | C1—C2—Co1—C8 | -144.7 (3) |
| C2—C1—C5—C4 | -0.2 (6) | C8—C7—Co1—C6 | 119.8 (6) |
| P1—C1—C5—C4 | 176.8 (4) | C8—C7—Co1—C1 | -147.6 (4) |
| Co1—C1—C5—C4 | -60.4 (4) | C6—C7—Co1—C1 | 92.7 (4) |
| C2—C1—C5—Co1 | 60.2 (4) | C8—C7—Co1—C10 | 80.9 (5) |
| P1—C1—C5—Co1 | -122.8 (4) | C6—C7—Co1—C10 | -38.8 (3) |
| C10—C6—C7—C8 | 0.7 (6) | C8—C7—Co1—C5 | 176.0 (4) |
| P2—C6—C7—C8 | -179.6 (4) | C6—C7—Co1—C5 | 56.2 (5) |
| Co1—C6—C7—C8 | -59.5 (4) | C8—C7—Co1—C2 | -103.4 (4) |
| C10—C6—C7—Co1 | 60.1 (4) | C6—C7—Co1—C2 | 136.8 (3) |
| P2—C6—C7—Co1 | -120.1 (4) | C8—C7—Co1—C3 | -65.3 (6) |
| C6—C7—C8—C9 | -1.0 (7) | C6—C7—Co1—C3 | 174.9 (3) |
| Co1—C7—C8—C9 | -58.7 (5) | C8—C7—Co1—C4 | -50 (3) |
| C6—C7—C8—Co1 | 57.7 (4) | C6—C7—Co1—C4 | -170 (3) |
| C7—C8—C9—C10 | 1.0 (8) | C8—C7—Co1—C9 | 36.4 (4) |
| Co1—C8—C9—C10 | -56.9 (5) | C6—C7—Co1—C9 | -83.4 (4) |
| C7—C8—C9—Co1 | 57.9 (5) | C6—C7—Co1—C8 | -119.8 (6) |
| C7—C6—C10—C9 | -0.1 (6) | C4—C3—Co1—C6 | -132 (3) |
| P2—C6—C10—C9 | -179.8 (4) | C2—C3—Co1—C6 | -14 (3) |
| Co1—C6—C10—C9 | 60.5 (4) | C4—C3—Co1—C1 | -81.5 (4) |
| C7—C6—C10—Co1 | -60.6 (4) | C2—C3—Co1—C1 | 37.4 (3) |
| P2—C6—C10—Co1 | 119.7 (4) | C4—C3—Co1—C10 | 57.4 (6) |
| C8—C9—C10—C6 | -0.6 (7) | C2—C3—Co1—C10 | 176.2 (4) |
| Co1—C9—C10—C6 | -59.0 (4) | C4—C3—Co1—C5 | -36.7 (3) |
| C8—C9—C10—Co1 | 58.5 (5) | C2—C3—Co1—C5 | 82.1 (4) |
| C16—C11—C12—C13 | -1.5 (10) | C4—C3—Co1—C2 | -118.9 (5) |
| P1—C11—C12—C13 | 175.0 (6) | C4—C3—Co1—C7 | 178.1 (4) |
| C11—C12—C13—C14 | -0.2 (11) | C2—C3—Co1—C7 | -63.0 (5) |

supplementary materials

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|-----------------|------------|---------------|------------|
| C12—C13—C14—C15 | 1.8 (11) | C2—C3—Co1—C4 | 118.9 (5) |
| C13—C14—C15—C16 | -1.7 (11) | C4—C3—Co1—C9 | 96.0 (4) |
| C14—C15—C16—C11 | 0.0 (10) | C2—C3—Co1—C9 | -145.1 (4) |
| C12—C11—C16—C15 | 1.6 (9) | C4—C3—Co1—C8 | 138.9 (4) |
| P1—C11—C16—C15 | -174.9 (5) | C2—C3—Co1—C8 | -102.2 (4) |
| C22—C17—C18—C19 | 1.9 (9) | C3—C4—Co1—C6 | 174.5 (4) |
| P1—C17—C18—C19 | -176.2 (5) | C5—C4—Co1—C6 | 53.3 (5) |
| C17—C18—C19—C20 | -0.1 (10) | C3—C4—Co1—C1 | 82.6 (4) |
| C18—C19—C20—C21 | -0.7 (11) | C5—C4—Co1—C1 | -38.6 (3) |
| C19—C20—C21—C22 | -0.4 (11) | C3—C4—Co1—C10 | -146.3 (4) |
| C20—C21—C22—C17 | 2.1 (10) | C5—C4—Co1—C10 | 92.5 (4) |
| C18—C17—C22—C21 | -2.9 (9) | C3—C4—Co1—C5 | 121.2 (5) |
| P1—C17—C22—C21 | 175.3 (5) | C3—C4—Co1—C2 | 38.0 (3) |
| C28—C23—C24—C25 | -0.5 (8) | C5—C4—Co1—C2 | -83.2 (4) |
| P2—C23—C24—C25 | 179.7 (4) | C3—C4—Co1—C7 | -17 (3) |
| C23—C24—C25—C26 | 1.2 (8) | C5—C4—Co1—C7 | -138 (3) |
| C24—C25—C26—C27 | -1.3 (9) | C5—C4—Co1—C3 | -121.2 (5) |
| C25—C26—C27—C28 | 0.7 (9) | C3—C4—Co1—C9 | -101.3 (4) |
| C24—C23—C28—C27 | 0.0 (8) | C5—C4—Co1—C9 | 137.5 (4) |
| P2—C23—C28—C27 | 179.8 (4) | C3—C4—Co1—C8 | -63.0 (5) |
| C26—C27—C28—C23 | -0.1 (9) | C5—C4—Co1—C8 | 175.9 (4) |
| C34—C29—C30—C31 | 0.5 (9) | C8—C9—Co1—C6 | -82.1 (4) |
| P2—C29—C30—C31 | -175.5 (5) | C10—C9—Co1—C6 | 38.4 (4) |
| C29—C30—C31—C32 | -0.8 (10) | C8—C9—Co1—C1 | -126 (4) |
| C30—C31—C32—C33 | 0.7 (11) | C10—C9—Co1—C1 | -5(4) |
| C31—C32—C33—C34 | -0.3 (12) | C8—C9—Co1—C10 | -120.5 (6) |
| C32—C33—C34—C29 | 0.0 (11) | C8—C9—Co1—C5 | 177.6 (3) |
| C30—C29—C34—C33 | -0.1 (10) | C10—C9—Co1—C5 | -61.9 (5) |
| P2—C29—C34—C33 | 175.9 (5) | C8—C9—Co1—C2 | 56.6 (6) |
| C10—C6—Co1—C1 | 139.1 (4) | C10—C9—Co1—C2 | 177.2 (4) |
| C7—C6—Co1—C1 | -103.0 (4) | C8—C9—Co1—C7 | -37.1 (4) |
| P2—C6—Co1—C1 | 16.5 (4) | C10—C9—Co1—C7 | 83.4 (4) |
| C7—C6—Co1—C10 | 117.9 (5) | C8—C9—Co1—C3 | 94.3 (4) |
| P2—C6—Co1—C10 | -122.6 (5) | C10—C9—Co1—C3 | -145.2 (4) |
| C10—C6—Co1—C5 | 95.0 (4) | C8—C9—Co1—C4 | 137.9 (4) |
| C7—C6—Co1—C5 | -147.2 (4) | C10—C9—Co1—C4 | -101.6 (4) |
| P2—C6—Co1—C5 | -27.6 (4) | C10—C9—Co1—C8 | 120.5 (6) |
| C10—C6—Co1—C2 | 176.4 (4) | C9—C8—Co1—C6 | 82.4 (4) |
| C7—C6—Co1—C2 | -65.7 (5) | C7—C8—Co1—C6 | -38.2 (4) |
| P2—C6—Co1—C2 | 53.8 (5) | C9—C8—Co1—C1 | 175.2 (3) |
| C10—C6—Co1—C7 | -117.9 (5) | C7—C8—Co1—C1 | 54.6 (6) |
| P2—C6—Co1—C7 | 119.5 (5) | C9—C8—Co1—C10 | 37.7 (4) |
| C10—C6—Co1—C3 | -171 (3) | C7—C8—Co1—C10 | -82.9 (4) |
| C7—C6—Co1—C3 | -53 (3) | C9—C8—Co1—C5 | -24 (3) |
| P2—C6—Co1—C3 | 66 (3) | C7—C8—Co1—C5 | -144 (3) |
| C10—C6—Co1—C4 | 60.7 (5) | C9—C8—Co1—C2 | -146.3 (4) |
| C7—C6—Co1—C4 | 178.6 (4) | C7—C8—Co1—C2 | 93.1 (4) |
| P2—C6—Co1—C4 | -61.8 (5) | C9—C8—Co1—C7 | 120.6 (6) |
| C10—C6—Co1—C9 | -38.2 (4) | C9—C8—Co1—C3 | -102.4 (4) |

| | | | |
|---------------|------------|----------------|------------|
| C7—C6—Co1—C9 | 79.6 (4) | C7—C8—Co1—C3 | 137.0 (4) |
| P2—C6—Co1—C9 | -160.8 (5) | C9—C8—Co1—C4 | -64.5 (5) |
| C10—C6—Co1—C8 | -80.8 (4) | C7—C8—Co1—C4 | 174.9 (4) |
| C7—C6—Co1—C8 | 37.1 (4) | C7—C8—Co1—C9 | -120.6 (6) |
| P2—C6—Co1—C8 | 156.6 (5) | C16—C11—P1—C17 | -111.8 (5) |
| C2—C1—Co1—C6 | 139.5 (3) | C12—C11—P1—C17 | 71.7 (5) |
| C5—C1—Co1—C6 | -102.8 (3) | C16—C11—P1—C1 | 144.6 (5) |
| P1—C1—Co1—C6 | 18.6 (4) | C12—C11—P1—C1 | -31.8 (6) |
| C2—C1—Co1—C10 | 177.4 (3) | C16—C11—P1—Pt1 | 13.7 (5) |
| C5—C1—Co1—C10 | -64.9 (4) | C12—C11—P1—Pt1 | -162.8 (5) |
| P1—C1—Co1—C10 | 56.4 (5) | C18—C17—P1—C11 | -8.5 (5) |
| C2—C1—Co1—C5 | -117.8 (4) | C22—C17—P1—C11 | 173.3 (4) |
| P1—C1—Co1—C5 | 121.3 (5) | C18—C17—P1—C1 | 94.4 (5) |
| C5—C1—Co1—C2 | 117.8 (4) | C22—C17—P1—C1 | -83.8 (4) |
| P1—C1—Co1—C2 | -120.9 (5) | C18—C17—P1—Pt1 | -135.3 (4) |
| C2—C1—Co1—C7 | 95.0 (3) | C22—C17—P1—Pt1 | 46.5 (5) |
| C5—C1—Co1—C7 | -147.2 (3) | C2—C1—P1—C11 | 126.1 (5) |
| P1—C1—Co1—C7 | -25.9 (4) | C5—C1—P1—C11 | -50.4 (5) |
| C2—C1—Co1—C3 | -36.9 (3) | Co1—C1—P1—C11 | -142.0 (4) |
| C5—C1—Co1—C3 | 80.9 (3) | C2—C1—P1—C17 | 15.4 (5) |
| P1—C1—Co1—C3 | -157.8 (4) | C5—C1—P1—C17 | -161.1 (5) |
| C2—C1—Co1—C4 | -80.0 (3) | Co1—C1—P1—C17 | 107.2 (4) |
| C5—C1—Co1—C4 | 37.7 (3) | C2—C1—P1—Pt1 | -108.2 (5) |
| P1—C1—Co1—C4 | 159.1 (4) | C5—C1—P1—Pt1 | 75.3 (5) |
| C2—C1—Co1—C9 | -178 (4) | Co1—C1—P1—Pt1 | -16.3 (4) |
| C5—C1—Co1—C9 | -60 (4) | P2—Pt1—P1—C11 | 104.7 (2) |
| P1—C1—Co1—C9 | 62 (4) | Cl2—Pt1—P1—C11 | -62.6 (4) |
| C2—C1—Co1—C8 | 60.2 (5) | Cl1—Pt1—P1—C11 | -71.8 (2) |
| C5—C1—Co1—C8 | 178.0 (4) | P2—Pt1—P1—C17 | -131.6 (2) |
| P1—C1—Co1—C8 | -60.7 (5) | Cl2—Pt1—P1—C17 | 61.1 (4) |
| C9—C10—Co1—C6 | -118.8 (6) | Cl1—Pt1—P1—C17 | 51.9 (2) |
| C6—C10—Co1—C1 | -61.7 (5) | P2—Pt1—P1—C1 | -13.8 (2) |
| C9—C10—Co1—C1 | 179.5 (4) | Cl2—Pt1—P1—C1 | 178.9 (3) |
| C6—C10—Co1—C5 | -101.2 (3) | Cl1—Pt1—P1—C1 | 169.7 (2) |
| C9—C10—Co1—C5 | 140.0 (4) | C28—C23—P2—C29 | -39.1 (5) |
| C6—C10—Co1—C2 | -37 (4) | C24—C23—P2—C29 | 140.6 (4) |
| C9—C10—Co1—C2 | -156 (3) | C28—C23—P2—C6 | 66.5 (5) |
| C6—C10—Co1—C7 | 39.0 (3) | C24—C23—P2—C6 | -113.7 (4) |
| C9—C10—Co1—C7 | -79.8 (4) | C28—C23—P2—Pt1 | -165.6 (4) |
| C6—C10—Co1—C3 | 178.9 (4) | C24—C23—P2—Pt1 | 14.2 (4) |
| C9—C10—Co1—C3 | 60.0 (6) | C30—C29—P2—C23 | -39.7 (5) |
| C6—C10—Co1—C4 | -144.8 (3) | C34—C29—P2—C23 | 144.4 (5) |
| C9—C10—Co1—C4 | 96.4 (4) | C30—C29—P2—C6 | -148.6 (5) |
| C6—C10—Co1—C9 | 118.8 (6) | C34—C29—P2—C6 | 35.5 (5) |
| C6—C10—Co1—C8 | 82.6 (4) | C30—C29—P2—Pt1 | 84.9 (5) |
| C9—C10—Co1—C8 | -36.2 (4) | C34—C29—P2—Pt1 | -91.0 (5) |
| C4—C5—Co1—C6 | -148.5 (3) | C10—C6—P2—C23 | -15.8 (5) |
| C1—C5—Co1—C6 | 92.7 (3) | C7—C6—P2—C23 | 164.4 (4) |
| C4—C5—Co1—C1 | 118.8 (4) | Co1—C6—P2—C23 | 74.8 (4) |

supplementary materials

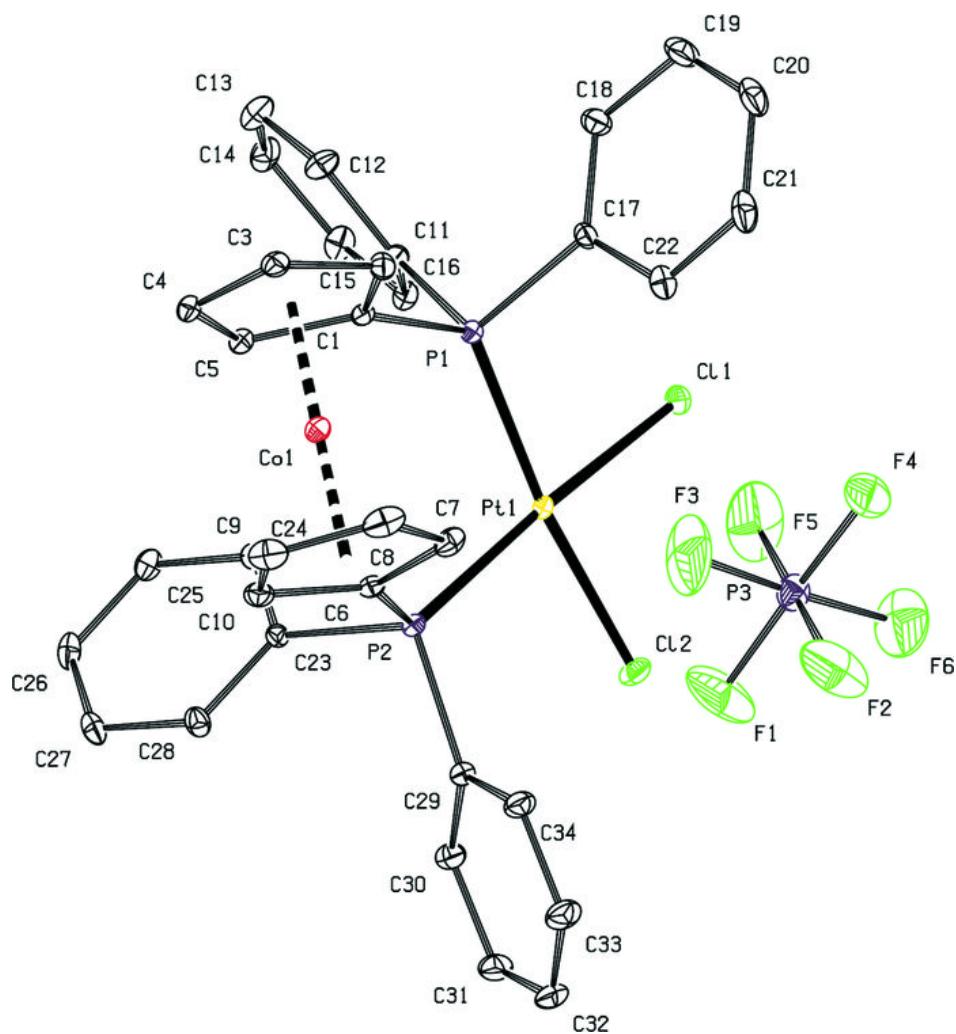
| | | | |
|---------------|------------|----------------|--------------|
| C4—C5—Co1—C10 | −104.0 (4) | C10—C6—P2—C29 | 93.9 (5) |
| C1—C5—Co1—C10 | 137.3 (3) | C7—C6—P2—C29 | −85.8 (5) |
| C4—C5—Co1—C2 | 80.1 (3) | Co1—C6—P2—C29 | −175.4 (3) |
| C1—C5—Co1—C2 | −38.7 (3) | C10—C6—P2—Pt1 | −140.8 (4) |
| C4—C5—Co1—C7 | 174.9 (4) | C7—C6—P2—Pt1 | 39.4 (5) |
| C1—C5—Co1—C7 | 56.1 (5) | Co1—C6—P2—Pt1 | −50.2 (4) |
| C4—C5—Co1—C3 | 36.3 (3) | P1—Pt1—P2—C23 | −77.79 (17) |
| C1—C5—Co1—C3 | −82.5 (3) | Cl2—Pt1—P2—C23 | 100.09 (17) |
| C1—C5—Co1—C4 | −118.8 (4) | Cl1—Pt1—P2—C23 | 66.8 (5) |
| C4—C5—Co1—C9 | −65.8 (4) | P1—Pt1—P2—C29 | 160.9 (2) |
| C1—C5—Co1—C9 | 175.4 (3) | Cl2—Pt1—P2—C29 | −21.2 (2) |
| C4—C5—Co1—C8 | −44 (3) | Cl1—Pt1—P2—C29 | −54.4 (5) |
| C1—C5—Co1—C8 | −163 (3) | P1—Pt1—P2—C6 | 43.48 (19) |
| C3—C2—Co1—C6 | 178.5 (3) | Cl2—Pt1—P2—C6 | −138.64 (19) |
| C1—C2—Co1—C6 | −61.0 (4) | Cl1—Pt1—P2—C6 | −171.9 (5) |

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···F2 ⁱ | 0.98 | 2.32 | 3.190 (11) | 148 |
| C4—H4···Cl1 ⁱⁱ | 0.98 | 2.80 | 3.448 (7) | 124 |
| C7—H7···F5 | 0.98 | 2.55 | 3.513 (14) | 168 |
| C12—H12···F6 ⁱⁱⁱ | 0.93 | 2.54 | 3.267 (11) | 135 |
| C14—H14···Cl2 ⁱⁱⁱ | 0.93 | 2.79 | 3.497 (8) | 134 |
| C16—H16···Cl1 | 0.93 | 2.80 | 3.454 (7) | 128 |
| C22—H22···F5 | 0.93 | 2.51 | 3.311 (11) | 145 |

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

Fig. 1



supplementary materials

Fig. 2

