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# {Bis[2-(diphenylphosphino)ethyl]phenylphosphine-$\kappa^3P,P',P''$}chloridoplatinium(II) hexafluoridophosphate

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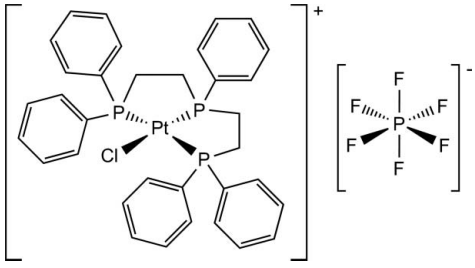
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.006 Å; disorder in solvent or counterion; $R$ factor = 0.020; $wR$ factor = 0.049; data-to-parameter ratio = 13.6.

In the title compound, $[PtCl(C_{34}H_{33}P_3)]PF_6$, the $Pt^{II}$ cation adopts a distorted square-planar $PtClP_3$ geometry, arising from the $P,P',P''$-tridentate triphos ligand and a chloride ion. Four of the F atoms of the $PF_6^-$ anion are disordered over two sets of positions in a 0.614 (17):0.386 (17) ratio.

## Related literature

The corresponding complex with a $Pd^{II}$ metal center is published concurently (Vorce *et al.*, 2009). The corresponding $Pt^{II}$ complex has been previously reported as a $CuCl_2^-$ salt (Fernadez *et al.*, 2005). The corresponding complexes with both $Pt^{II}$ and $Pd^{II}$ have been previously reported as chloride and diphenyltetrachloridostannate(IV) salts (Sevillano *et al.*, 1999*a*; Garcia-Seijo *et al.*, 2001; Housecroft *et al.*, 1990). For other group 10–triphos complexes, see: Sevillano *et al.* (1999*b*); Müller *et al.* (2000); Aizawa *et al.* (2002); Bertinsson *et al.* (1983); Autissier *et al.* (2005); Fernandez *et al.* (2005); King *et al.* (1971).




## Experimental

### Crystal data

$[PtCl(C_{34}H_{33}P_3)]PF_6$ $M_r$ = 910.02
Monoclinic, $P2_1/c$
$a$ = 11.3870 (11) Å
$b$ = 19.6221 (18) Å
$c$ = 16.4439 (16) Å
$\beta$ = 107.528 (3)°
$V$ = 3503.6 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 4.32 mm$^{-1}$
$T$ = 298 K
0.50 × 0.30 × 0.10 mm

### Data collection

Bruker SMART X2S diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008*a*)
$T_{min}$ = 0.21, $T_{max}$ = 0.65
21968 measured reflections
6155 independent reflections
5269 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.049
$S$ = 1.03
6155 reflections
452 parameters
204 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.41 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Pt1—P2 | 2.2095 (8) | Pt1—P1 | 2.3185 (8) |
| Pt1—P3 | 2.3007 (8) | Pt1—Cl1 | 2.3434 (8) |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2993).

## References

Aizawa, S., Sone, Y., Kawamoto, T., Yamada, S. & Nakamura, M. (2002). *Inorg. Chim. Acta*, **338**, 235–239.
Autissier, V., Brockman, E., Clegg, W., Harrington, R. W. & Henderson, R. A. (2005). *J. Organomet. Chem.* **690**, 1763–1771.
Bertinsson, G.-I. (1983). *Acta Cryst.* C**39**, 563–567.
Bruker (2008). *APEX2*, *SAINT* and *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fernandez, D., Garcia-Seijo, M. I., Sevillano, P., Castineiras, A. & Garcia-Fernandez, M. E. (2005). *Inorg. Chim. Acta*, **358**, 2575–2584.
Garcia-Seijo, M. I., Castineiras, A., Mahieu, B., Janosi, L., Berente, Z., Kollar, L. & Garcia-Fernandez, M. E. (2001). *Polyhedron*, **20**, 855–868.
Housecroft, C. E., Shaykh, B. A. M., Rheingold, A. L. & Haggerty, B. S. (1990). *Acta Cryst.* C**46**, 1549–1551.
King, R. B., Kapoor, P. N. & Kapoor, R. N. (1971). *Inorg. Chem.* **10**, 1841–1850.
Müller, T. E., Grosche, M., Herdtweck, E., Pleier, A.-K., Walter, E. & Yaw-Kai, Y. (2000). *Organometallics*, **19**, 170–183.
Sevillano, P., Habtemariam, A., Parsons, S., Castineiras, A., Garcia, M. E. & Sadler, P. J. (1999*a*). *J. Chem. Soc. Dalton Trans.* pp. 2861–2870.
Sevillano, P., Habtemariam, A., Parsons, S., Castineiras, A., Garcia, M. E. & Sadler, P. J. (1999*b*). *Polyhedron*, **18**, 383–389.
Sheldrick, G. M. (2008*a*). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008*b*). *Acta Cryst.* A**64**, 112–122.
Vorce, P. R., Miller, S. M. & Helm, M. L. (2009). *Acta Cryst.* E**65**, m792.

# supplementary materials

*Acta Cryst.* (2009). E**65**, m793 [ **doi:10.1107/S1600536809022405** ]

# {Bis[2-(diphenylphosphino)ethyl]phenylphosphine-$\kappa^3P,P',P''$}chloridoplatinium(II) hexafluoridophosphate

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## Comment

The crystal structure of the title compound, (I), consists of a $[Pt(triphos)Cl]^+$ cation and disordered $PF_6^-$ anion (Fig. 1). The cation shows a distorted square planar geometry (Table 1) around the metal center with a non-coordinating $PF_6^-$ anion.

## Experimental

The synthesis of (**I**) by a previously reported proceedure (King, *et al.*, 1971). Crystals where grown by slow solvent evaporation of a saturated dichloromethane solution of (**I**).

## Figures

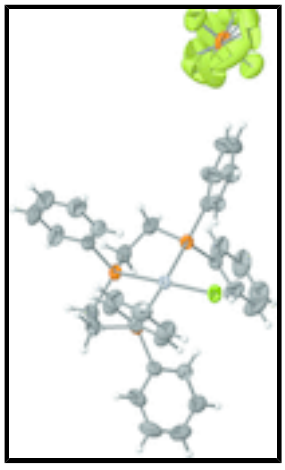


Fig. 1. The molecular structure of (I), with 50% probability displacement ellipsoids.

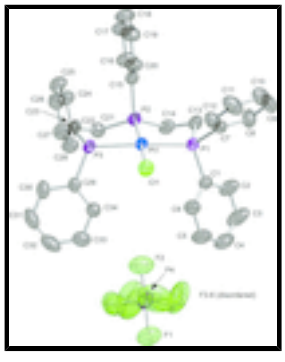


Fig. 2. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

## {Bis[2-(diphenylphosphino)ethyl]phenylphosphine- $\kappa^3P,P',P''$}chloridoplatinium(II) hexafluoridophosphate

*Crystal data*

| | |
|---|---|
| $[PtCl(C_{34}H_{33}P_3)]PF_6$ | $F_{000}$ = 1784 |
| $M_r$ = 910.02 | $D_x$ = 1.725 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 9957 reflections |
| $a$ = 11.3870 (11) Å | θ = 2.5–25.1º |
| $b$ = 19.6221 (18) Å | μ = 4.32 mm$^{-1}$ |
| $c$ = 16.4439 (16) Å | $T$ = 298 K |
| β = 107.528 (3)º | Plate, colorless |
| $V$ = 3503.6 (6) Å$^3$ | 0.50 × 0.30 × 0.10 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART X2S diffractometer | 6155 independent reflections |
| Monochromator: graphite | 5269 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 8.33 pixels mm$^{-1}$ | $R_{int}$ = 0.025 |
| $T$ = 298 K | $\theta_{max}$ = 25.1º |
| ω scans | $\theta_{min}$ = 2.8º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2008a) | $h$ = −13→13 |
| $T_{min}$ = 0.21, $T_{max}$ = 0.65 | $k$ = −18→23 |
| 21968 measured reflections | $l$ = −19→19 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.020 | H-atom parameters constrained |
| $wR(F^2)$ = 0.049 | $w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 1.641P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.03 | $(\Delta/\sigma)_{max}$ = 0.002 |
| 6155 reflections | $\Delta\rho_{max}$ = 0.58 e Å$^{-3}$ |
| 452 parameters | $\Delta\rho_{min}$ = −0.41 e Å$^{-3}$ |
| 204 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct 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**. The $PF_6$ anion is disordered, showing alternate positions of the 4 *F* atoms F3—F6 when rotated about the axis F1—P4—F2. A second orientation for these equatorial positions was located. Based on the thermal parameters, additional positions are indicated, but were not modeled. To improve the quality of the fit for this anion, distance restraints (*SHELX* SADI) were added for the P–*F* bonds, as well as for the *F*–*F* interatomic distances. These account for 156 of the 204 restraints applied. The remaining restraints (ISOR) were applied to the anisotropic displacement parameters for the fluorine atoms.

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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pt1 | 0.139852 (10) | 0.364806 (6) | 0.374003 (7) | 0.03173 (5) | |
| Cl1 | 0.31867 (8) | 0.35123 (5) | 0.48942 (5) | 0.0498 (2) | |
| P1 | 0.22200 (7) | 0.43573 (4) | 0.29227 (5) | 0.03695 (19) | |
| P2 | −0.03648 (7) | 0.37743 (4) | 0.27189 (5) | 0.03518 (19) | |
| P3 | 0.03774 (7) | 0.28264 (4) | 0.42630 (5) | 0.03706 (19) | |
| C1 | 0.3286 (3) | 0.39017 (18) | 0.2487 (2) | 0.0417 (8) | |
| C2 | 0.3950 (4) | 0.3357 (2) | 0.2925 (3) | 0.0696 (12) | |
| H2 | 0.3851 | 0.3227 | 0.3444 | 0.084* | |
| C3 | 0.4758 (5) | 0.3003 (3) | 0.2602 (4) | 0.0929 (17) | |
| H3 | 0.5209 | 0.2641 | 0.2909 | 0.111* | |
| C4 | 0.4896 (4) | 0.3182 (3) | 0.1838 (3) | 0.0811 (14) | |
| H4 | 0.5422 | 0.2933 | 0.1614 | 0.097* | |
| C5 | 0.4268 (4) | 0.3724 (3) | 0.1397 (3) | 0.0809 (15) | |
| H5 | 0.4382 | 0.3850 | 0.0881 | 0.097* | |
| C6 | 0.3458 (4) | 0.4088 (2) | 0.1716 (2) | 0.0662 (12) | |
| H6 | 0.3030 | 0.4457 | 0.1413 | 0.079* | |
| C7 | 0.2923 (3) | 0.51580 (17) | 0.3367 (2) | 0.0448 (8) | |
| C8 | 0.3091 (4) | 0.5681 (2) | 0.2843 (3) | 0.0690 (12) | |
| H8 | 0.2889 | 0.5616 | 0.2257 | 0.083* | |
| C9 | 0.3563 (5) | 0.6303 (2) | 0.3202 (4) | 0.0815 (15) | |
| H9 | 0.3673 | 0.6653 | 0.2852 | 0.098* | |
| C10 | 0.3863 (4) | 0.6405 (2) | 0.4054 (4) | 0.0774 (15) | |
| H10 | 0.4162 | 0.6827 | 0.4283 | 0.093* | |
| C11 | 0.3726 (4) | 0.5886 (2) | 0.4579 (3) | 0.0774 (14) | |
| H11 | 0.3950 | 0.5954 | 0.5166 | 0.093* | |
| C12 | 0.3255 (3) | 0.5262 (2) | 0.4237 (3) | 0.0587 (10) | |
| H12 | 0.3162 | 0.4913 | 0.4595 | 0.070* | |

| | | | | | |
|---|---|---|---|---|---|
| C13 | 0.0924 (3) | 0.46082 (19) | 0.2000 (2) | 0.0480 (9) | |
| H13A | 0.0534 | 0.5012 | 0.2141 | 0.058* | |
| H13B | 0.1226 | 0.4718 | 0.1524 | 0.058* | |
| C14 | −0.0024 (3) | 0.40301 (19) | 0.1745 (2) | 0.0459 (8) | |
| H14A | 0.0311 | 0.3649 | 0.1510 | 0.055* | |
| H14B | −0.0766 | 0.4188 | 0.1320 | 0.055* | |
| C15 | −0.1372 (3) | 0.44123 (17) | 0.2947 (2) | 0.0392 (8) | |
| C16 | −0.2526 (3) | 0.4525 (2) | 0.2376 (2) | 0.0612 (11) | |
| H16 | −0.2769 | 0.4292 | 0.1860 | 0.073* | |
| C17 | −0.3320 (4) | 0.4987 (2) | 0.2575 (3) | 0.0777 (13) | |
| H17 | −0.4097 | 0.5061 | 0.2192 | 0.093* | |
| C18 | −0.2964 (4) | 0.5334 (2) | 0.3334 (3) | 0.0718 (12) | |
| H18 | −0.3501 | 0.5642 | 0.3462 | 0.086* | |
| C19 | −0.1830 (4) | 0.5230 (2) | 0.3901 (3) | 0.0655 (11) | |
| H19 | −0.1593 | 0.5468 | 0.4413 | 0.079* | |
| C20 | −0.1031 (3) | 0.47681 (18) | 0.3711 (2) | 0.0512 (9) | |
| H20 | −0.0258 | 0.4696 | 0.4100 | 0.061* | |
| C21 | −0.1212 (3) | 0.29792 (17) | 0.2618 (2) | 0.0446 (8) | |
| H21A | −0.2052 | 0.3041 | 0.2255 | 0.054* | |
| H21B | −0.0824 | 0.2631 | 0.2368 | 0.054* | |
| C22 | −0.1201 (3) | 0.27699 (19) | 0.3519 (2) | 0.0500 (9) | |
| H22A | −0.1502 | 0.2307 | 0.3510 | 0.060* | |
| H22B | −0.1743 | 0.3067 | 0.3713 | 0.060* | |
| C23 | 0.0305 (3) | 0.29942 (17) | 0.5330 (2) | 0.0413 (8) | |
| C24 | −0.0603 (3) | 0.3399 (2) | 0.5480 (2) | 0.0529 (9) | |
| H24 | −0.1274 | 0.3533 | 0.5027 | 0.063* | |
| C25 | −0.0518 (4) | 0.3605 (2) | 0.6305 (3) | 0.0605 (11) | |
| H25 | −0.1135 | 0.3874 | 0.6402 | 0.073* | |
| C26 | 0.0467 (4) | 0.3415 (2) | 0.6974 (2) | 0.0590 (10) | |
| H26 | 0.0533 | 0.3564 | 0.7523 | 0.071* | |
| C27 | 0.1362 (4) | 0.3003 (2) | 0.6833 (2) | 0.0614 (11) | |
| H27 | 0.2024 | 0.2865 | 0.7290 | 0.074* | |
| C28 | 0.1287 (3) | 0.2791 (2) | 0.6017 (2) | 0.0538 (9) | |
| H28 | 0.1896 | 0.2512 | 0.5929 | 0.065* | |
| C29 | 0.1039 (3) | 0.19806 (16) | 0.42953 (19) | 0.0387 (8) | |
| C30 | 0.0425 (4) | 0.14216 (19) | 0.4497 (2) | 0.0539 (10) | |
| H30 | −0.0322 | 0.1483 | 0.4609 | 0.065* | |
| C31 | 0.0923 (5) | 0.0778 (2) | 0.4532 (3) | 0.0677 (12) | |
| H31 | 0.0515 | 0.0407 | 0.4673 | 0.081* | |
| C32 | 0.2015 (4) | 0.0680 (2) | 0.4359 (3) | 0.0675 (12) | |
| H32 | 0.2343 | 0.0244 | 0.4381 | 0.081* | |
| C33 | 0.2626 (4) | 0.1225 (2) | 0.4153 (3) | 0.0610 (11) | |
| H33 | 0.3362 | 0.1157 | 0.4029 | 0.073* | |
| C34 | 0.2149 (3) | 0.18766 (18) | 0.4131 (2) | 0.0456 (8) | |
| H34 | 0.2575 | 0.2246 | 0.4005 | 0.055* | |
| P4 | 0.33951 (10) | 0.86107 (6) | 0.53542 (7) | 0.0655 (3) | |
| F1 | 0.2344 (3) | 0.91309 (17) | 0.5407 (2) | 0.1331 (13) | |
| F2 | 0.4424 (3) | 0.81198 (16) | 0.5283 (2) | 0.1263 (12) | |
| F3 | 0.4311 (7) | 0.8949 (6) | 0.6137 (6) | 0.170 (6) | 0.614 (17) |

| | | | | | |
|---|---|---|---|---|---|
| F4 | 0.2458 (8) | 0.8302 (5) | 0.4551 (7) | 0.181 (7) | 0.614 (17) |
| F5 | 0.3788 (11) | 0.9131 (4) | 0.4771 (7) | 0.143 (6) | 0.614 (17) |
| F6 | 0.2992 (7) | 0.8122 (5) | 0.5916 (7) | 0.196 (7) | 0.614 (17) |
| F3' | 0.3623 (16) | 0.8459 (7) | 0.6302 (5) | 0.170 (11) | 0.386 (17) |
| F4' | 0.3028 (14) | 0.8713 (10) | 0.4399 (5) | 0.184 (10) | 0.386 (17) |
| F5' | 0.4294 (9) | 0.9199 (4) | 0.5545 (15) | 0.153 (11) | 0.386 (17) |
| F6' | 0.2434 (11) | 0.8018 (5) | 0.5150 (11) | 0.141 (9) | 0.386 (17) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pt1 | 0.02685 (7) | 0.03558 (8) | 0.03213 (7) | −0.00116 (5) | 0.00792 (5) | 0.00172 (5) |
| Cl1 | 0.0352 (4) | 0.0585 (6) | 0.0467 (5) | −0.0016 (4) | −0.0013 (4) | 0.0038 (4) |
| P1 | 0.0324 (4) | 0.0385 (5) | 0.0422 (5) | 0.0009 (4) | 0.0147 (4) | 0.0056 (4) |
| P2 | 0.0290 (4) | 0.0438 (5) | 0.0311 (4) | 0.0000 (4) | 0.0066 (3) | −0.0002 (3) |
| P3 | 0.0322 (4) | 0.0416 (5) | 0.0385 (4) | −0.0023 (4) | 0.0124 (4) | 0.0045 (4) |
| C1 | 0.0343 (17) | 0.046 (2) | 0.0465 (19) | −0.0013 (15) | 0.0144 (15) | −0.0008 (16) |
| C2 | 0.069 (3) | 0.069 (3) | 0.086 (3) | 0.022 (2) | 0.047 (3) | 0.023 (2) |
| C3 | 0.095 (4) | 0.080 (4) | 0.126 (4) | 0.042 (3) | 0.067 (4) | 0.029 (3) |
| C4 | 0.069 (3) | 0.085 (4) | 0.103 (4) | 0.011 (3) | 0.046 (3) | −0.021 (3) |
| C5 | 0.061 (3) | 0.134 (5) | 0.056 (3) | 0.015 (3) | 0.029 (2) | −0.004 (3) |
| C6 | 0.057 (2) | 0.095 (3) | 0.051 (2) | 0.021 (2) | 0.023 (2) | 0.009 (2) |
| C7 | 0.0338 (18) | 0.039 (2) | 0.064 (2) | −0.0003 (15) | 0.0188 (17) | 0.0049 (17) |
| C8 | 0.081 (3) | 0.051 (3) | 0.087 (3) | −0.012 (2) | 0.043 (3) | 0.004 (2) |
| C9 | 0.083 (3) | 0.046 (3) | 0.122 (5) | −0.012 (2) | 0.041 (3) | 0.014 (3) |
| C10 | 0.047 (2) | 0.049 (3) | 0.122 (4) | −0.014 (2) | 0.003 (3) | −0.006 (3) |
| C11 | 0.063 (3) | 0.063 (3) | 0.084 (3) | −0.006 (2) | −0.014 (2) | −0.005 (3) |
| C12 | 0.049 (2) | 0.048 (2) | 0.068 (3) | −0.0065 (18) | 0.0007 (19) | 0.0046 (19) |
| C13 | 0.0418 (19) | 0.057 (2) | 0.048 (2) | 0.0080 (17) | 0.0177 (16) | 0.0167 (17) |
| C14 | 0.0408 (18) | 0.063 (2) | 0.0335 (17) | 0.0071 (18) | 0.0111 (14) | 0.0050 (16) |
| C15 | 0.0340 (17) | 0.042 (2) | 0.0423 (18) | 0.0025 (15) | 0.0124 (15) | 0.0026 (15) |
| C16 | 0.044 (2) | 0.074 (3) | 0.058 (2) | 0.008 (2) | 0.0042 (18) | −0.010 (2) |
| C17 | 0.045 (2) | 0.084 (3) | 0.094 (3) | 0.020 (2) | 0.006 (2) | −0.006 (3) |
| C18 | 0.057 (3) | 0.064 (3) | 0.098 (3) | 0.015 (2) | 0.028 (3) | −0.015 (3) |
| C19 | 0.066 (3) | 0.063 (3) | 0.067 (3) | 0.008 (2) | 0.019 (2) | −0.017 (2) |
| C20 | 0.045 (2) | 0.052 (2) | 0.053 (2) | 0.0059 (17) | 0.0090 (17) | −0.0046 (18) |
| C21 | 0.0377 (18) | 0.044 (2) | 0.0468 (19) | −0.0053 (15) | 0.0043 (15) | −0.0068 (16) |
| C22 | 0.0346 (18) | 0.055 (2) | 0.058 (2) | −0.0089 (16) | 0.0104 (16) | 0.0066 (18) |
| C23 | 0.0398 (18) | 0.045 (2) | 0.0432 (18) | −0.0014 (15) | 0.0189 (15) | 0.0061 (15) |
| C24 | 0.047 (2) | 0.063 (2) | 0.051 (2) | 0.0083 (19) | 0.0199 (18) | 0.0037 (19) |
| C25 | 0.060 (3) | 0.069 (3) | 0.062 (3) | 0.009 (2) | 0.032 (2) | 0.000 (2) |
| C26 | 0.076 (3) | 0.062 (3) | 0.046 (2) | 0.002 (2) | 0.027 (2) | 0.0018 (19) |
| C27 | 0.067 (3) | 0.073 (3) | 0.042 (2) | 0.012 (2) | 0.0129 (19) | 0.0082 (19) |
| C28 | 0.055 (2) | 0.062 (3) | 0.046 (2) | 0.0145 (19) | 0.0190 (18) | 0.0076 (18) |
| C29 | 0.0413 (18) | 0.040 (2) | 0.0339 (16) | −0.0049 (15) | 0.0096 (14) | 0.0008 (14) |
| C30 | 0.060 (2) | 0.053 (3) | 0.051 (2) | −0.0172 (19) | 0.0205 (19) | −0.0012 (18) |
| C31 | 0.096 (4) | 0.043 (3) | 0.061 (3) | −0.020 (2) | 0.020 (2) | 0.0018 (19) |
| C32 | 0.086 (3) | 0.042 (2) | 0.063 (3) | 0.008 (2) | 0.005 (2) | −0.007 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C33 | 0.057 (2) | 0.053 (3) | 0.069 (3) | 0.007 (2) | 0.012 (2) | −0.007 (2) |
| C34 | 0.045 (2) | 0.043 (2) | 0.049 (2) | −0.0006 (16) | 0.0130 (16) | 0.0008 (16) |
| P4 | 0.0518 (6) | 0.0859 (9) | 0.0608 (7) | 0.0022 (6) | 0.0199 (5) | 0.0198 (6) |
| F1 | 0.085 (2) | 0.135 (3) | 0.193 (4) | 0.031 (2) | 0.062 (2) | 0.027 (3) |
| F2 | 0.100 (2) | 0.108 (3) | 0.178 (3) | 0.0275 (19) | 0.052 (2) | −0.005 (2) |
| F3 | 0.082 (5) | 0.309 (16) | 0.115 (7) | −0.058 (7) | 0.025 (4) | −0.069 (8) |
| F4 | 0.133 (9) | 0.174 (11) | 0.166 (11) | 0.000 (7) | −0.061 (7) | −0.044 (8) |
| F5 | 0.200 (12) | 0.121 (8) | 0.155 (10) | 0.039 (7) | 0.122 (9) | 0.062 (7) |
| F6 | 0.121 (6) | 0.265 (13) | 0.210 (13) | −0.036 (7) | 0.061 (8) | 0.170 (11) |
| F3' | 0.27 (3) | 0.174 (15) | 0.051 (5) | 0.124 (16) | 0.023 (9) | 0.000 (7) |
| F4' | 0.183 (16) | 0.31 (3) | 0.047 (6) | −0.042 (14) | 0.010 (8) | 0.053 (10) |
| F5' | 0.083 (8) | 0.077 (7) | 0.31 (3) | −0.036 (5) | 0.079 (15) | −0.040 (13) |
| F6' | 0.163 (15) | 0.110 (10) | 0.198 (19) | −0.074 (10) | 0.130 (15) | −0.031 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Pt1—P2 | 2.2095 (8) | C17—C18 | 1.371 (6) |
| Pt1—P3 | 2.3007 (8) | C17—H17 | 0.9300 |
| Pt1—P1 | 2.3185 (8) | C18—C19 | 1.361 (6) |
| Pt1—Cl1 | 2.3434 (8) | C18—H18 | 0.9300 |
| P1—C7 | 1.814 (4) | C19—C20 | 1.384 (5) |
| P1—C1 | 1.819 (3) | C19—H19 | 0.9300 |
| P1—C13 | 1.836 (3) | C20—H20 | 0.9300 |
| P2—C15 | 1.812 (3) | C21—C22 | 1.535 (5) |
| P2—C21 | 1.815 (3) | C21—H21A | 0.9700 |
| P2—C14 | 1.828 (3) | C21—H21B | 0.9700 |
| P3—C23 | 1.812 (3) | C22—H22A | 0.9700 |
| P3—C29 | 1.817 (3) | C22—H22B | 0.9700 |
| P3—C22 | 1.848 (3) | C23—C24 | 1.383 (5) |
| C1—C2 | 1.380 (5) | C23—C28 | 1.387 (5) |
| C1—C6 | 1.389 (5) | C24—C25 | 1.392 (5) |
| C2—C3 | 1.381 (6) | C24—H24 | 0.9300 |
| C2—H2 | 0.9300 | C25—C26 | 1.365 (6) |
| C3—C4 | 1.359 (6) | C25—H25 | 0.9300 |
| C3—H3 | 0.9300 | C26—C27 | 1.375 (5) |
| C4—C5 | 1.362 (6) | C26—H26 | 0.9300 |
| C4—H4 | 0.9300 | C27—C28 | 1.382 (5) |
| C5—C6 | 1.388 (6) | C27—H27 | 0.9300 |
| C5—H5 | 0.9300 | C28—H28 | 0.9300 |
| C6—H6 | 0.9300 | C29—C34 | 1.385 (4) |
| C7—C12 | 1.381 (5) | C29—C30 | 1.393 (5) |
| C7—C8 | 1.390 (5) | C30—C31 | 1.379 (5) |
| C8—C9 | 1.390 (6) | C30—H30 | 0.9300 |
| C8—H8 | 0.9300 | C31—C32 | 1.370 (6) |
| C9—C10 | 1.352 (7) | C31—H31 | 0.9300 |
| C9—H9 | 0.9300 | C32—C33 | 1.372 (6) |
| C10—C11 | 1.375 (6) | C32—H32 | 0.9300 |
| C10—H10 | 0.9300 | C33—C34 | 1.385 (5) |
| C11—C12 | 1.386 (5) | C33—H33 | 0.9300 |

| | | | |
|---|---|---|---|
| C11—H11 | 0.9300 | C34—H34 | 0.9300 |
| C12—H12 | 0.9300 | P4—F6 | 1.496 (5) |
| C13—C14 | 1.535 (5) | P4—F5' | 1.512 (8) |
| C13—H13A | 0.9700 | P4—F4' | 1.512 (8) |
| C13—H13B | 0.9700 | P4—F3' | 1.530 (8) |
| C14—H14A | 0.9700 | P4—F3 | 1.542 (7) |
| C14—H14B | 0.9700 | P4—F2 | 1.548 (3) |
| C15—C16 | 1.383 (5) | P4—F4 | 1.549 (6) |
| C15—C20 | 1.387 (5) | P4—F5 | 1.556 (6) |
| C16—C17 | 1.387 (5) | P4—F6' | 1.563 (8) |
| C16—H16 | 0.9300 | P4—F1 | 1.595 (3) |
| P2—Pt1—P3 | 85.22 (3) | C18—C19—C20 | 119.7 (4) |
| P2—Pt1—P1 | 85.71 (3) | C18—C19—H19 | 120.1 |
| P3—Pt1—P1 | 167.13 (3) | C20—C19—H19 | 120.1 |
| P2—Pt1—Cl1 | 175.83 (3) | C19—C20—C15 | 120.7 (3) |
| P3—Pt1—Cl1 | 91.79 (3) | C19—C20—H20 | 119.7 |
| P1—Pt1—Cl1 | 97.69 (3) | C15—C20—H20 | 119.7 |
| C7—P1—C1 | 108.56 (15) | C22—C21—P2 | 107.0 (2) |
| C7—P1—C13 | 104.36 (16) | C22—C21—H21A | 110.3 |
| C1—P1—C13 | 105.78 (16) | P2—C21—H21A | 110.3 |
| C7—P1—Pt1 | 119.51 (12) | C22—C21—H21B | 110.3 |
| C1—P1—Pt1 | 111.53 (12) | P2—C21—H21B | 110.3 |
| C13—P1—Pt1 | 105.99 (11) | H21A—C21—H21B | 108.6 |
| C15—P2—C21 | 105.12 (16) | C21—C22—P3 | 110.3 (2) |
| C15—P2—C14 | 107.82 (16) | C21—C22—H22A | 109.6 |
| C21—P2—C14 | 113.75 (16) | P3—C22—H22A | 109.6 |
| C15—P2—Pt1 | 114.03 (11) | C21—C22—H22B | 109.6 |
| C21—P2—Pt1 | 108.04 (11) | P3—C22—H22B | 109.6 |
| C14—P2—Pt1 | 108.22 (11) | H22A—C22—H22B | 108.1 |
| C23—P3—C29 | 106.08 (15) | C24—C23—C28 | 118.9 (3) |
| C23—P3—C22 | 109.46 (16) | C24—C23—P3 | 122.1 (3) |
| C29—P3—C22 | 106.05 (16) | C28—C23—P3 | 118.4 (3) |
| C23—P3—Pt1 | 114.22 (11) | C23—C24—C25 | 120.3 (4) |
| C29—P3—Pt1 | 113.54 (11) | C23—C24—H24 | 119.9 |
| C22—P3—Pt1 | 107.16 (11) | C25—C24—H24 | 119.9 |
| C2—C1—C6 | 118.3 (3) | C26—C25—C24 | 120.4 (4) |
| C2—C1—P1 | 120.0 (3) | C26—C25—H25 | 119.8 |
| C6—C1—P1 | 121.6 (3) | C24—C25—H25 | 119.8 |
| C1—C2—C3 | 120.9 (4) | C25—C26—C27 | 119.7 (4) |
| C1—C2—H2 | 119.6 | C25—C26—H26 | 120.1 |
| C3—C2—H2 | 119.6 | C27—C26—H26 | 120.1 |
| C4—C3—C2 | 120.1 (4) | C26—C27—C28 | 120.6 (4) |
| C4—C3—H3 | 120.0 | C26—C27—H27 | 119.7 |
| C2—C3—H3 | 120.0 | C28—C27—H27 | 119.7 |
| C3—C4—C5 | 120.4 (4) | C27—C28—C23 | 120.2 (3) |
| C3—C4—H4 | 119.8 | C27—C28—H28 | 119.9 |
| C5—C4—H4 | 119.8 | C23—C28—H28 | 119.9 |
| C4—C5—C6 | 120.2 (4) | C34—C29—C30 | 118.9 (3) |
| C4—C5—H5 | 119.9 | C34—C29—P3 | 121.6 (3) |

| | | | |
|---|---|---|---|
| C6—C5—H5 | 119.9 | C30—C29—P3 | 119.5 (3) |
| C5—C6—C1 | 120.1 (4) | C31—C30—C29 | 120.1 (4) |
| C5—C6—H6 | 119.9 | C31—C30—H30 | 120.0 |
| C1—C6—H6 | 119.9 | C29—C30—H30 | 120.0 |
| C12—C7—C8 | 119.1 (4) | C32—C31—C30 | 120.5 (4) |
| C12—C7—P1 | 119.7 (3) | C32—C31—H31 | 119.8 |
| C8—C7—P1 | 121.1 (3) | C30—C31—H31 | 119.8 |
| C7—C8—C9 | 119.5 (4) | C31—C32—C33 | 120.1 (4) |
| C7—C8—H8 | 120.3 | C31—C32—H32 | 119.9 |
| C9—C8—H8 | 120.3 | C33—C32—H32 | 119.9 |
| C10—C9—C8 | 121.0 (4) | C32—C33—C34 | 120.1 (4) |
| C10—C9—H9 | 119.5 | C32—C33—H33 | 119.9 |
| C8—C9—H9 | 119.5 | C34—C33—H33 | 119.9 |
| C9—C10—C11 | 119.9 (4) | C29—C34—C33 | 120.3 (3) |
| C9—C10—H10 | 120.0 | C29—C34—H34 | 119.9 |
| C11—C10—H10 | 120.0 | C33—C34—H34 | 119.9 |
| C10—C11—C12 | 120.2 (5) | F5'—P4—F4' | 94.2 (8) |
| C10—C11—H11 | 119.9 | F5'—P4—F3' | 92.3 (7) |
| C12—C11—H11 | 119.9 | F4'—P4—F3' | 173.1 (8) |
| C7—C12—C11 | 120.2 (4) | F6—P4—F3 | 90.9 (5) |
| C7—C12—H12 | 119.9 | F6—P4—F2 | 91.6 (4) |
| C11—C12—H12 | 119.9 | F5'—P4—F2 | 90.6 (4) |
| C14—C13—P1 | 110.6 (2) | F4'—P4—F2 | 89.0 (5) |
| C14—C13—H13A | 109.5 | F3'—P4—F2 | 93.2 (4) |
| P1—C13—H13A | 109.5 | F3—P4—F2 | 89.6 (4) |
| C14—C13—H13B | 109.5 | F6—P4—F4 | 90.9 (5) |
| P1—C13—H13B | 109.5 | F3—P4—F4 | 177.5 (5) |
| H13A—C13—H13B | 108.1 | F2—P4—F4 | 92.0 (3) |
| C13—C14—P2 | 106.3 (2) | F6—P4—F5 | 178.6 (5) |
| C13—C14—H14A | 110.5 | F3—P4—F5 | 89.1 (4) |
| P2—C14—H14A | 110.5 | F2—P4—F5 | 89.8 (3) |
| C13—C14—H14B | 110.5 | F4—P4—F5 | 89.0 (5) |
| P2—C14—H14B | 110.5 | F5'—P4—F6' | 178.3 (6) |
| H14A—C14—H14B | 108.7 | F4'—P4—F6' | 85.3 (8) |
| C16—C15—C20 | 118.9 (3) | F3'—P4—F6' | 88.1 (6) |
| C16—C15—P2 | 120.1 (3) | F2—P4—F6' | 91.0 (4) |
| C20—C15—P2 | 120.9 (3) | F6—P4—F1 | 90.1 (4) |
| C15—C16—C17 | 119.9 (4) | F5'—P4—F1 | 88.4 (4) |
| C15—C16—H16 | 120.1 | F4'—P4—F1 | 89.7 (5) |
| C17—C16—H16 | 120.1 | F3'—P4—F1 | 88.2 (4) |
| C18—C17—C16 | 120.2 (4) | F3—P4—F1 | 90.5 (4) |
| C18—C17—H17 | 119.9 | F2—P4—F1 | 178.3 (2) |
| C16—C17—H17 | 119.9 | F4—P4—F1 | 87.8 (3) |
| C19—C18—C17 | 120.6 (4) | F5—P4—F1 | 88.5 (3) |
| C19—C18—H18 | 119.7 | F6'—P4—F1 | 90.0 (4) |
| C17—C18—H18 | 119.7 | | |

**Fig. 1**

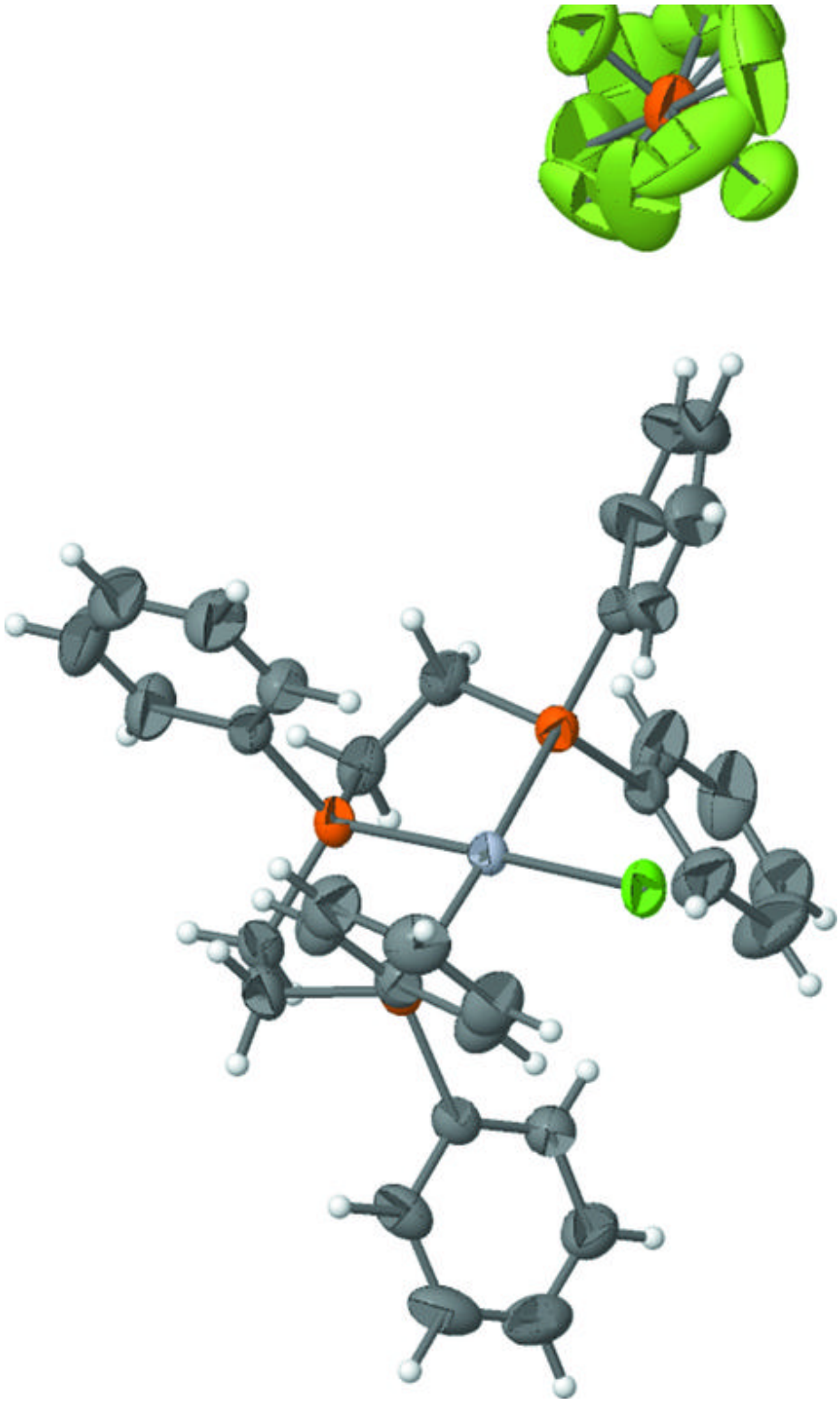
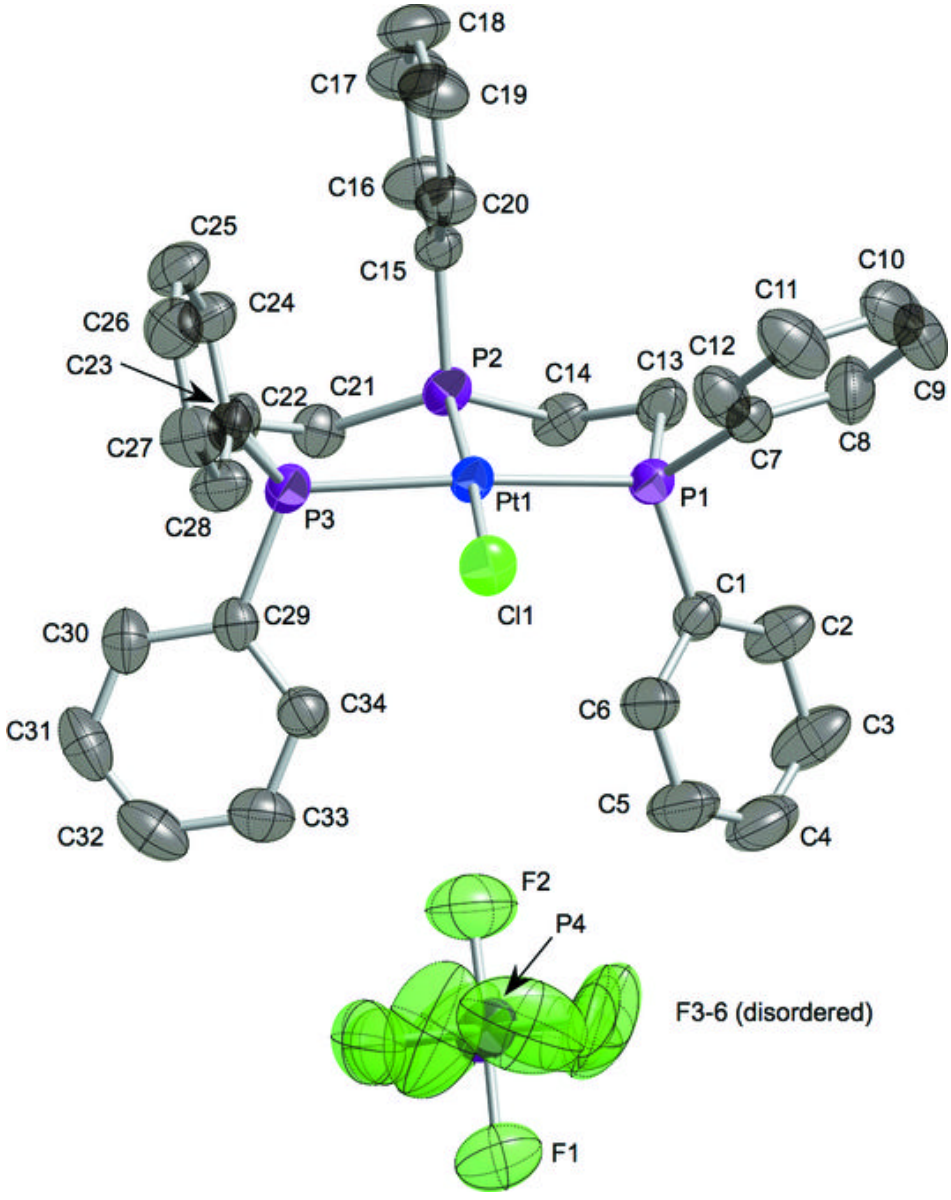


**Fig. 2**


C18
C17
C19
C16
C20
C25
C15
C10
C11
C24
C26
C12
C23
P2
C14
C13
C9
C22
C21
C27
C8
C7
Pt1
P1
C28
P3
C1
Cl1
C30
C29
C2
C34
C6
C31
C3
C5
C33
C32
C4
F2
P4
F3-6 (disordered)
F1