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(Acetonitrile-κN)(2,2′:6′,2″-terpyridyl-$\kappa^3 N$)palladium(II)] bis(hexafluorophosphate)

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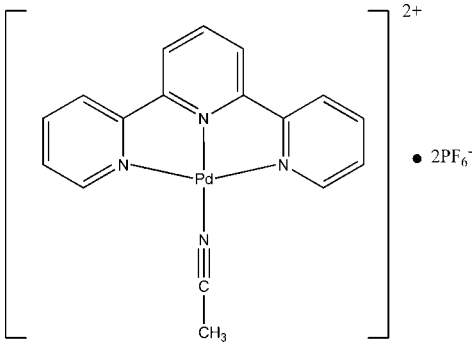
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.142; data-to-parameter ratio = 16.7.

In the title compound, $[Pd(C_{15}H_{11}N_3)(C_2H_3N)](PF_6)_2$, the Pd atom is four-coordinated by a tridentate chelating 2,2′:6′,2″-terpyridine ligand and an acetonitrile ligand in a square-planar geometry. The cations and hexafluoridophosphate anions are connected together *via* anion–π interactions [P—F$\cdots\pi$ = 3.063 (5) and 3.076 (6) Å] and C—H$\cdots$F hydrogen bonds to form alternating layers along the *b* axis.

Related literature

For literature on the 2,2′:6′,2″-terpyridine complexes of palladium(II) and platinum(II), see: Angle *et al.* (2006); Onoda *et al.* (2003); Roszak *et al.* (1996).



Experimental

Crystal data

$[Pd(C_{15}H_{11}N_3)(C_2H_3N)](PF_6)_2$
M_r = 670.66
Monoclinic, $P2_1/c$
a = 13.1073 (3) Å
b = 11.8840 (3) Å
c = 14.6085 (4) Å
β = 97.810 (1)°
V = 2254.42 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 273 (2) K
0.30 × 0.24 × 0.22 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.738, T_{max} = 0.797
16715 measured reflections
5449 independent reflections
4503 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.142
S = 1.06
5449 reflections
326 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.023 (3)	Pd1—N3	2.026 (3)
Pd1—N2	1.929 (3)	Pd1—N4	2.025 (3)
N2—Pd1—N1	81.0 (1)	N2—Pd1—N3	80.9 (1)
N2—Pd1—N4	179.6 (1)	N1—Pd1—N3	161.9 (1)

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C15—H15$\cdots$F9^{i}	0.93	2.37	3.213 (6)	151
C14—H14$\cdots$F10^{i}	0.93	2.47	3.268 (9)	143
C13—H13$\cdots$F12^{ii}	0.93	2.45	3.142 (7)	131
C7—H7$\cdots$F5^{iii}	0.93	2.40	3.326 (7)	173
C3—H3$\cdots$F3^{iv}	0.93	2.47	3.363 (7)	162
P1—F2$\cdots Cg1$		2.95	3.062 (5)	122
P2—F12$\cdots Cg2^{v}$		2.97	3.075 (6)	122

Symmetry codes: (i) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y, -z+1$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $x-1, y, z$. Notes: *Cg*1 and *Cg*2 are the centroids of rings Pd1/N1/C5/C6/N2 and Pd1/N2/C10/C11/N3, respectively.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2287).

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supplementary materials

Acta Cryst. (2007). E**63**, m2029 [**doi:10.1107/S160053680703070X**]

(Acetonitrile-κN)(2,2':6',2''-terpyridyl-$\kappa^3 N$)palladium(II)] bis(hexafluorophosphate)

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Comment

The 2,2':6',2''-terpyridine complexes of palladium(II) and platinum(II) have the metal centers in a square-planar geometry (Angle *et al.*, 2006; Onoda *et al.*, 2003; Roszak *et al.*, 1996). The title compound also displays square-planar coordination, with four N atoms from terpy and acetonitrile molecule (Fig. 1). The crystal structure comprises alternating layers of cations and anions as represented in Fig. 2. The compound packs by an anion–π interaction (P1—F2···*Cg*1 3.063 (5) Å [*Cg*1 is the centroid of the ring system Pd1, N1, C5, C6, N2; P2—F12···*Cg*2 3.076 (6) Å, *Cg*2 is the centroid of the ring system Pd1, N2, C10, C11, N3] and hydrogen bonds involving hexafluorophosphate anions (C—H···F). Non-classical hydrogen bonds that connect cations, anions and coordinated acetonitrile molecules are detailed in Table 2.

Experimental

(2,2':6',2''-Terpyridyl-$\kappa^3 N$)dinitratopalladium (46.4 mg, 0.10 mmol) was dissolved in water (5 ml), and a tenfold excess of potassium hexafluorophosphate was added, which resulted in the immediate deposition deep yellow microcrystals. The crystals were filtered, washed with a minimum amount of cold water and dried under vacuum (quantative yield of 59.6 mg). Crystals were obtained by the vapor diffusion of diethyl ether into a 2 m*M* solution in acetonitrile.

Refinement

The aromatic H atoms were constrained to an ideal geometry, with C—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The methyl H atoms were rotated to fit the electron density, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). The largest peak and deepest hole on the final difference Fourier map corresponds to 0.84 and −0.61 e.Å^{-3}, and were located 1.14 and 0.42Å from the F12 and F10 atoms.

Figures

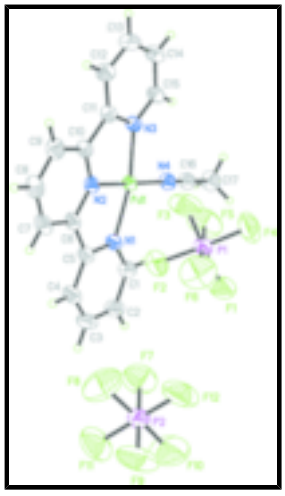


Fig. 1. **Figure 1**. A view of the title compound (I), showing 30% probability displacement ellipsoids and the atom numbering scheme.

(Acetonitrile-κ*N*)(2,2':6',2''-terpyridyl-κ^3*N*)palladium(II)] bis(hexafluorophosphate)

Crystal data

$[Pd(C_{15}H_{11}N_3)(C_2H_3N)](PF_6)_2$	F_{000} = 1312
M_r = 670.66	D_x = 1.976 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 8518 reflections
a = 13.1073 (3) Å	θ = 2.2–28.3º
b = 11.8840 (3) Å	μ = 1.08 mm^{-1}
c = 14.6085 (4) Å	T = 273 (2) K
β = 97.8100 (10)º	Block, yellow
V = 2254.42 (10) Å^3	0.30 × 0.24 × 0.22 mm
Z = 4	

Data collection

Bruker SMART diffractometer	5449 independent reflections
Radiation source: sealed tube	4503 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
T = 273(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −15→17
T_{min} = 0.738, T_{max} = 0.797	k = −15→15
16715 measured reflections	l = −19→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + (0.0789P)^2 + 2.9852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
5449 reflections	$\Delta\rho_{max} = 0.84$ e Å^{-3}
326 parameters	$\Delta\rho_{min} = -0.61$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.76117 (2)	0.28974 (2)	0.599820 (18)	0.04089 (12)
N1	0.6996 (2)	0.3828 (3)	0.6946 (2)	0.0479 (7)
N2	0.7149 (2)	0.1693 (3)	0.6726 (2)	0.0426 (6)
N3	0.8072 (2)	0.1568 (3)	0.5289 (2)	0.0444 (6)
N4	0.8108 (3)	0.4156 (3)	0.5235 (2)	0.0527 (8)
C1	0.6934 (3)	0.4957 (4)	0.6996 (3)	0.0570 (10)
H1	0.7211	0.5393	0.6562	0.068*
C2	0.6472 (4)	0.5483 (5)	0.7672 (4)	0.0691 (12)
H2	0.6433	0.6263	0.7692	0.083*
C3	0.6070 (4)	0.4841 (5)	0.8313 (3)	0.0695 (13)
H3	0.5765	0.5187	0.8779	0.083*
C4	0.6115 (3)	0.3684 (5)	0.8272 (3)	0.0617 (11)
H4	0.5833	0.3241	0.8699	0.074*
C5	0.6589 (3)	0.3196 (4)	0.7584 (3)	0.0498 (8)
C6	0.6679 (3)	0.1969 (4)	0.7459 (3)	0.0489 (9)
C7	0.6330 (4)	0.1121 (4)	0.7987 (3)	0.0622 (11)
H7	0.5998	0.1286	0.8494	0.075*
C8	0.6495 (4)	0.0009 (4)	0.7734 (3)	0.0691 (13)

H8	0.6265	−0.0574	0.8079	0.083*
C9	0.6985 (4)	−0.0243 (4)	0.6990 (3)	0.0615 (11)
H9	0.7095	−0.0988	0.6832	0.074*
C10	0.7317 (3)	0.0635 (3)	0.6473 (3)	0.0475 (8)
C11	0.7857 (3)	0.0558 (3)	0.5664 (3)	0.0468 (8)
C12	0.8143 (4)	−0.0446 (4)	0.5296 (3)	0.0594 (10)
H12	0.8001	−0.1127	0.5567	0.071*
C13	0.8644 (4)	−0.0430 (4)	0.4523 (4)	0.0664 (12)
H13	0.8837	−0.1098	0.4263	0.080*
C14	0.8852 (4)	0.0591 (4)	0.4143 (3)	0.0648 (11)
H14	0.9185	0.0619	0.3621	0.078*
C15	0.8562 (3)	0.1575 (4)	0.4544 (3)	0.0533 (9)
H15	0.8713	0.2261	0.4287	0.064*
C16	0.8393 (3)	0.4869 (4)	0.4829 (3)	0.0554 (9)
C17	0.8762 (4)	0.5793 (4)	0.4315 (4)	0.0729 (13)
H17A	0.8209	0.6312	0.4137	0.109*
H17B	0.9011	0.5506	0.3772	0.109*
H17C	0.9310	0.6174	0.4695	0.109*
P1	0.42931 (10)	0.28021 (9)	0.51579 (8)	0.0546 (3)
F1	0.3845 (4)	0.4019 (3)	0.5203 (3)	0.1248 (16)
F2	0.4705 (4)	0.2847 (4)	0.6212 (3)	0.1263 (17)
F3	0.4664 (6)	0.1569 (4)	0.5074 (4)	0.177 (3)
F4	0.3944 (6)	0.2746 (5)	0.4096 (3)	0.158 (3)
F5	0.5332 (4)	0.3245 (6)	0.4898 (4)	0.158 (2)
F6	0.3290 (4)	0.2329 (6)	0.5489 (5)	0.160 (2)
P2	0.02951 (11)	0.19057 (12)	0.77715 (10)	0.0668 (3)
F7	0.1387 (4)	0.2137 (5)	0.7471 (4)	0.142 (2)
F8	0.0705 (5)	0.0699 (4)	0.8046 (5)	0.169 (2)
F9	−0.0789 (4)	0.1664 (6)	0.8057 (4)	0.162 (2)
F10	−0.0074 (9)	0.3078 (6)	0.7566 (6)	0.237 (5)
F11	0.0641 (5)	0.2300 (6)	0.8785 (4)	0.156 (2)
F12	−0.0095 (4)	0.1471 (8)	0.6798 (4)	0.222 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.04320 (18)	0.04512 (18)	0.03571 (17)	−0.00289 (10)	0.01025 (11)	0.00267 (10)
N1	0.0457 (16)	0.0548 (18)	0.0442 (16)	0.0007 (13)	0.0104 (13)	−0.0044 (14)
N2	0.0403 (15)	0.0500 (16)	0.0381 (15)	−0.0042 (12)	0.0075 (11)	0.0078 (12)
N3	0.0465 (16)	0.0477 (16)	0.0404 (15)	−0.0032 (13)	0.0104 (12)	0.0006 (12)
N4	0.060 (2)	0.0489 (18)	0.0509 (18)	−0.0043 (15)	0.0158 (15)	0.0032 (14)
C1	0.059 (2)	0.055 (2)	0.059 (2)	0.0008 (18)	0.0123 (19)	−0.0036 (19)
C2	0.074 (3)	0.066 (3)	0.068 (3)	0.007 (2)	0.014 (2)	−0.016 (2)
C3	0.062 (3)	0.087 (3)	0.062 (3)	0.003 (2)	0.017 (2)	−0.025 (2)
C4	0.052 (2)	0.089 (3)	0.046 (2)	−0.004 (2)	0.0154 (17)	−0.007 (2)
C5	0.045 (2)	0.064 (2)	0.0416 (19)	−0.0035 (17)	0.0073 (15)	−0.0025 (17)
C6	0.045 (2)	0.065 (2)	0.0379 (18)	−0.0058 (16)	0.0086 (15)	0.0039 (16)
C7	0.062 (3)	0.082 (3)	0.046 (2)	−0.011 (2)	0.0207 (18)	0.011 (2)

C8	0.080 (3)	0.071 (3)	0.059 (3)	−0.016 (2)	0.018 (2)	0.019 (2)
C9	0.073 (3)	0.054 (2)	0.059 (2)	−0.012 (2)	0.014 (2)	0.0103 (19)
C10	0.051 (2)	0.050 (2)	0.0421 (18)	−0.0074 (16)	0.0079 (15)	0.0032 (15)
C11	0.049 (2)	0.0482 (19)	0.0426 (18)	−0.0057 (15)	0.0057 (15)	0.0004 (15)
C12	0.066 (3)	0.049 (2)	0.063 (3)	−0.0027 (19)	0.009 (2)	−0.0033 (19)
C13	0.070 (3)	0.061 (3)	0.071 (3)	0.004 (2)	0.021 (2)	−0.014 (2)
C14	0.066 (3)	0.077 (3)	0.056 (2)	−0.001 (2)	0.025 (2)	−0.009 (2)
C15	0.053 (2)	0.061 (2)	0.049 (2)	−0.0060 (18)	0.0181 (17)	−0.0010 (18)
C16	0.063 (2)	0.051 (2)	0.055 (2)	−0.0025 (18)	0.0167 (18)	0.0043 (18)
C17	0.083 (3)	0.065 (3)	0.074 (3)	−0.013 (2)	0.022 (2)	0.016 (2)
P1	0.0650 (7)	0.0540 (6)	0.0473 (6)	−0.0014 (5)	0.0168 (5)	−0.0016 (4)
F1	0.197 (5)	0.083 (2)	0.103 (3)	0.043 (3)	0.051 (3)	0.006 (2)
F2	0.132 (4)	0.175 (5)	0.067 (2)	0.031 (3)	−0.001 (2)	−0.009 (2)
F3	0.344 (9)	0.075 (3)	0.137 (4)	0.073 (4)	0.126 (5)	0.025 (3)
F4	0.256 (7)	0.143 (5)	0.063 (2)	0.043 (4)	−0.019 (3)	−0.013 (2)
F5	0.137 (4)	0.197 (5)	0.158 (5)	−0.049 (4)	0.092 (4)	−0.011 (4)
F6	0.095 (3)	0.179 (5)	0.214 (6)	−0.044 (3)	0.054 (4)	0.012 (5)
P2	0.0668 (8)	0.0756 (8)	0.0582 (7)	0.0143 (6)	0.0093 (6)	−0.0119 (6)
F7	0.114 (4)	0.171 (6)	0.150 (5)	−0.014 (3)	0.050 (3)	−0.007 (3)
F8	0.164 (5)	0.096 (3)	0.247 (7)	0.030 (3)	0.030 (4)	0.008 (4)
F9	0.095 (3)	0.249 (6)	0.153 (4)	−0.027 (4)	0.058 (3)	−0.093 (5)
F10	0.367 (12)	0.145 (5)	0.225 (8)	0.141 (7)	0.138 (8)	0.061 (5)
F11	0.146 (4)	0.230 (6)	0.087 (3)	−0.021 (4)	−0.004 (3)	−0.046 (4)
F12	0.126 (4)	0.430 (12)	0.100 (3)	0.089 (6)	−0.015 (3)	−0.124 (6)

Geometric parameters (Å, °)

Pd1—N1	2.023 (3)	C9—H9	0.9300
Pd1—N2	1.929 (3)	C10—C11	1.461 (6)
Pd1—N3	2.026 (3)	C11—C12	1.381 (6)
Pd1—N4	2.025 (3)	C12—C13	1.381 (7)
N1—C1	1.346 (5)	C12—H12	0.9300
N1—C5	1.362 (5)	C13—C14	1.377 (7)
N2—C10	1.338 (5)	C13—H13	0.9300
N2—C6	1.346 (5)	C14—C15	1.383 (6)
N3—C15	1.337 (5)	C14—H14	0.9300
N3—C11	1.365 (5)	C15—H15	0.9300
N4—C16	1.126 (5)	C16—C17	1.451 (6)
C1—C2	1.377 (6)	C17—H17A	0.9600
C1—H1	0.9300	C17—H17B	0.9600
C2—C3	1.367 (8)	C17—H17C	0.9600
C2—H2	0.9300	P1—F3	1.554 (4)
C3—C4	1.379 (7)	P1—F5	1.555 (4)
C3—H3	0.9300	P1—F4	1.558 (5)
C4—C5	1.379 (6)	P1—F2	1.561 (4)
C4—H4	0.9300	P1—F6	1.566 (5)
C5—C6	1.477 (6)	P1—F1	1.566 (4)
C6—C7	1.384 (6)	P2—F10	1.491 (6)
C7—C8	1.397 (7)	P2—F12	1.533 (5)

C7—H7	0.9300	P2—F9	1.561 (5)
C8—C9	1.369 (7)	P2—F11	1.561 (5)
C8—H8	0.9300	P2—F8	1.565 (5)
C9—C10	1.391 (5)	P2—F7	1.578 (5)
N2—Pd1—N1	81.0 (1)	C11—C12—C13	119.4 (4)
N2—Pd1—N4	179.6 (1)	C11—C12—H12	120.3
N1—Pd1—N4	99.2 (1)	C13—C12—H12	120.3
N2—Pd1—N3	80.9 (1)	C14—C13—C12	118.9 (4)
N1—Pd1—N3	161.9 (1)	C14—C13—H13	120.5
N4—Pd1—N3	98.9 (1)	C12—C13—H13	120.5
C1—N1—C5	118.7 (4)	C13—C14—C15	119.6 (4)
C1—N1—Pd1	127.9 (3)	C13—C14—H14	120.2
C5—N1—Pd1	113.4 (3)	C15—C14—H14	120.2
C10—N2—C6	123.9 (3)	N3—C15—C14	122.0 (4)
C10—N2—Pd1	118.0 (2)	N3—C15—H15	119.0
C6—N2—Pd1	118.0 (3)	C14—C15—H15	119.0
C15—N3—C11	118.7 (3)	N4—C16—C17	179.5 (5)
C15—N3—Pd1	128.4 (3)	C16—C17—H17A	109.5
C11—N3—Pd1	112.9 (2)	C16—C17—H17B	109.5
C16—N4—Pd1	178.3 (4)	H17A—C17—H17B	109.5
N1—C1—C2	121.8 (4)	C16—C17—H17C	109.5
N1—C1—H1	119.1	H17A—C17—H17C	109.5
C2—C1—H1	119.1	H17B—C17—H17C	109.5
C3—C2—C1	119.1 (5)	F3—P1—F5	90.3 (4)
C3—C2—H2	120.4	F3—P1—F4	86.2 (3)
C1—C2—H2	120.4	F5—P1—F4	85.4 (4)
C2—C3—C4	120.2 (4)	F3—P1—F2	92.3 (3)
C2—C3—H3	119.9	F5—P1—F2	91.8 (3)
C4—C3—H3	119.9	F4—P1—F2	176.8 (4)
C3—C4—C5	118.5 (5)	F3—P1—F6	88.3 (4)
C3—C4—H4	120.7	F5—P1—F6	175.8 (4)
C5—C4—H4	120.7	F4—P1—F6	98.5 (4)
N1—C5—C4	121.6 (4)	F2—P1—F6	84.3 (3)
N1—C5—C6	114.5 (3)	F3—P1—F1	176.0 (4)
C4—C5—C6	123.8 (4)	F5—P1—F1	92.5 (3)
N2—C6—C7	119.2 (4)	F4—P1—F1	91.2 (3)
N2—C6—C5	113.1 (3)	F2—P1—F1	90.5 (3)
C7—C6—C5	127.7 (4)	F6—P1—F1	89.0 (3)
C6—C7—C8	117.8 (4)	F10—P2—F12	94.0 (5)
C6—C7—H7	121.1	F10—P2—F9	86.8 (5)
C8—C7—H7	121.1	F12—P2—F9	89.1 (3)
C9—C8—C7	121.5 (4)	F10—P2—F11	87.4 (5)
C9—C8—H8	119.2	F12—P2—F11	176.4 (5)
C7—C8—H8	119.2	F9—P2—F11	87.7 (3)
C8—C9—C10	118.8 (4)	F10—P2—F8	176.7 (5)
C8—C9—H9	120.6	F12—P2—F8	89.3 (4)
C10—C9—H9	120.6	F9—P2—F8	93.2 (4)
N2—C10—C9	118.7 (4)	F11—P2—F8	89.2 (4)
N2—C10—C11	113.5 (3)	F10—P2—F7	93.6 (5)

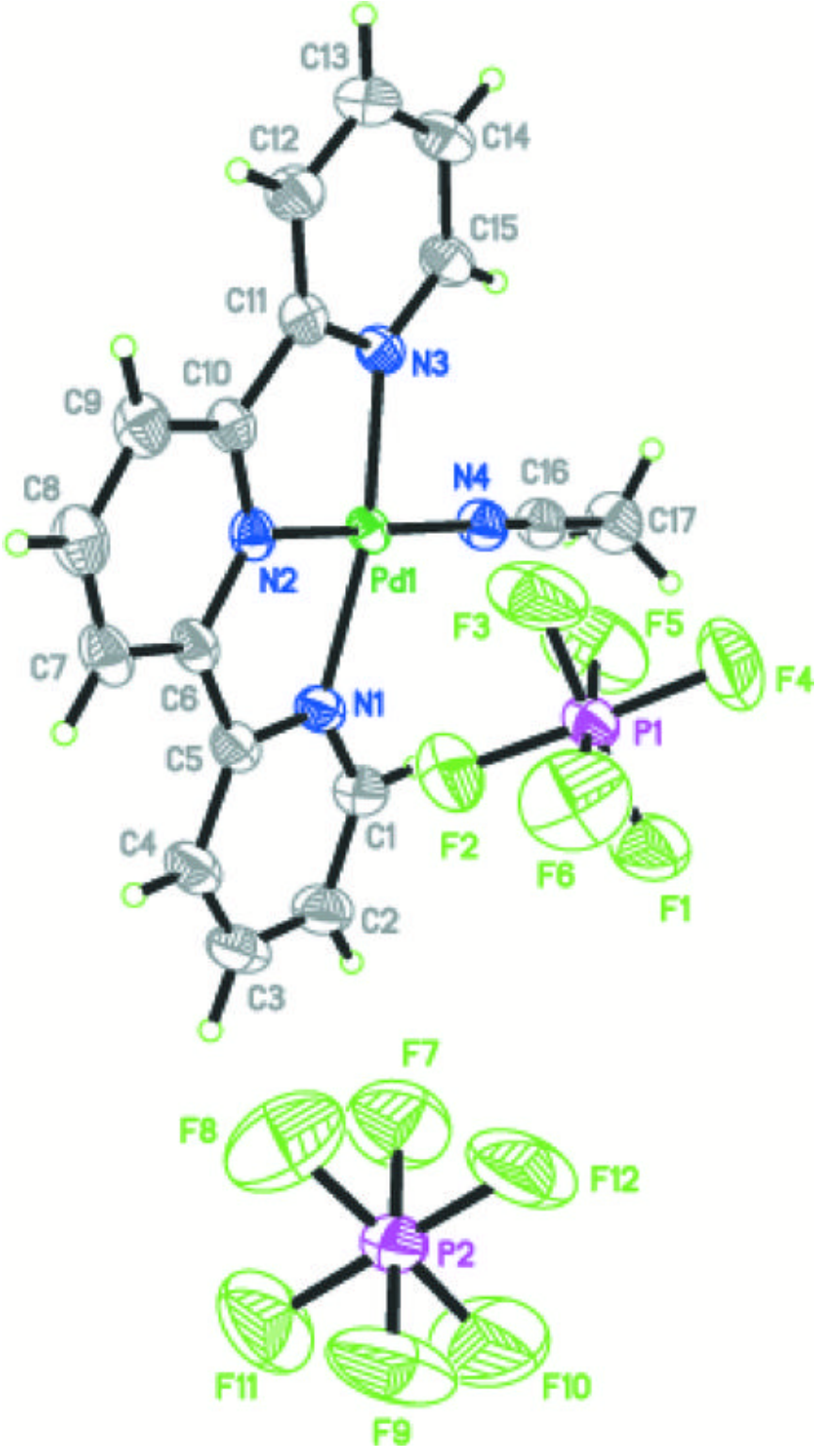
C9—C10—C11	127.8 (4)	F12—P2—F7	90.1 (4)
N3—C11—C12	121.5 (4)	F9—P2—F7	179.1 (3)
N3—C11—C10	114.8 (3)	F11—P2—F7	93.1 (3)
C12—C11—C10	123.8 (4)	F8—P2—F7	86.4 (3)
N2—Pd1—N1—C1	−178.6 (4)	Pd1—N2—C6—C5	0.3 (4)
N4—Pd1—N1—C1	1.7 (4)	N1—C5—C6—N2	−0.3 (5)
N3—Pd1—N1—C1	−178.3 (4)	C4—C5—C6—N2	178.4 (4)
N2—Pd1—N1—C5	0.0 (3)	N1—C5—C6—C7	−179.3 (4)
N4—Pd1—N1—C5	−179.7 (3)	C4—C5—C6—C7	−0.6 (7)
N3—Pd1—N1—C5	0.3 (6)	N2—C6—C7—C8	0.5 (7)
N1—Pd1—N2—C10	179.9 (3)	C5—C6—C7—C8	179.5 (4)
N3—Pd1—N2—C10	0.0 (3)	C6—C7—C8—C9	0.1 (8)
N1—Pd1—N2—C6	−0.1 (3)	C7—C8—C9—C10	−0.6 (8)
N3—Pd1—N2—C6	180.0 (3)	C6—N2—C10—C9	0.2 (6)
N2—Pd1—N3—C15	−179.3 (4)	Pd1—N2—C10—C9	−179.8 (3)
N1—Pd1—N3—C15	−179.7 (4)	C6—N2—C10—C11	−179.1 (3)
N4—Pd1—N3—C15	0.3 (4)	Pd1—N2—C10—C11	0.9 (5)
N2—Pd1—N3—C11	−1.0 (3)	C8—C9—C10—N2	0.4 (7)
N1—Pd1—N3—C11	−1.3 (6)	C8—C9—C10—C11	179.6 (4)
N4—Pd1—N3—C11	178.7 (3)	C15—N3—C11—C12	0.8 (6)
C5—N1—C1—C2	0.0 (7)	Pd1—N3—C11—C12	−177.7 (3)
Pd1—N1—C1—C2	178.6 (3)	C15—N3—C11—C10	−179.8 (4)
N1—C1—C2—C3	0.4 (8)	Pd1—N3—C11—C10	1.7 (4)
C1—C2—C3—C4	−1.0 (8)	N2—C10—C11—N3	−1.7 (5)
C2—C3—C4—C5	1.2 (8)	C9—C10—C11—N3	179.1 (4)
C1—N1—C5—C4	0.2 (6)	N2—C10—C11—C12	177.7 (4)
Pd1—N1—C5—C4	−178.6 (3)	C9—C10—C11—C12	−1.5 (7)
C1—N1—C5—C6	178.9 (4)	N3—C11—C12—C13	−1.2 (7)
Pd1—N1—C5—C6	0.2 (4)	C10—C11—C12—C13	179.4 (4)
C3—C4—C5—N1	−0.8 (7)	C11—C12—C13—C14	0.6 (8)
C3—C4—C5—C6	−179.4 (4)	C12—C13—C14—C15	0.3 (8)
C10—N2—C6—C7	−0.7 (6)	C11—N3—C15—C14	0.2 (6)
Pd1—N2—C6—C7	179.4 (3)	Pd1—N3—C15—C14	178.4 (3)
C10—N2—C6—C5	−179.8 (3)	C13—C14—C15—N3	−0.7 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···F9^{i}	0.93	2.37	3.213 (6)	151
C14—H14···F10^{i}	0.93	2.47	3.268 (9)	143
C13—H13···F12^{ii}	0.93	2.45	3.142 (7)	131
C7—H7···F5^{iii}	0.93	2.40	3.326 (7)	173
C3—H3···F3^{iv}	0.93	2.47	3.363 (7)	162
P1—F2···Cg1	?	2.95	3.062 (5)	122.3 (3)
P2—F12···Cg2^{v}	?	2.97	3.075 (6)	121.7 (3)

Symmetry codes: (i) *x*+1, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*, −*y*+1/2, *z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+3/2; (v) *x*−1, *y*, *z*.

Fig. 1


C13
C12
C14
C15
C11
N3
C10
C9
C8
N4
C16
C17
N2
Pd1
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F4
C7
C6
N1
P1
C5
C1
F2
F6
F1
C4
C2
C3
F7
F8
F12
P2
F11
F10
F9