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Crystal structure of bis(2-{1-[(E)-(4-fluorobenzyl)-imino]ethyl}phenolato-$\kappa^2 N,O$)palladium(II)

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The asymmetric unit of the title complex, [Pd(C$_{15}$H$_{13}$FNO)$_2$], contains one half of the molecule with the Pd^{II} cation lying on an inversion centre and is coordinated by the bidentate Schiff base anion. The geometry around the cationic Pd^{II} centre is distorted square planar, chelated by the imine N- and phenolate O-donor atoms of the two Schiff base ligands. The N- and O-donor atoms of the two ligands are mutually *trans*, with Pd—N and Pd—O bond lengths of 2.028 (2) and 1.9770 (18) Å, respectively. The fluorophenyl ring is tilted away from the coordination plane and makes a dihedral angle of 66.2 (2)° with the phenolate ring. In the crystal, molecules are linked into chains along the [101] direction by weak C—H$\cdots$O hydrogen bonds. Weak $\pi-\pi$ interactions with centroid–centroid distances of 4.079 (2) Å stack the molecules along c.

1. Chemical context

Schiff bases represent one of the most widely utilized classes of ligands in coordination chemistry and the chemistry of Schiff bases is still an area of increasing interest (Canali & Sherrigton, 1999). The Pd^{II} and Ni^{II} complexes of Schiff bases have attracted much attention as they play important roles in bioinorganic chemistry and may provide the basis for models of active sites of biological systems (Malik *et al.*, 2013) or act as catalysts (Shahnaz *et al.*, 2013). The title compound, [Pd(C$_{15}$H$_{13}$FNO)$_2$], is related to the previously reported compound bis{2-[(E)-(4-fluorobenzyl)iminomethyl]pheno-lato-$\kappa^2 N,O^1$}nickel(II) (Mohd Tajuddin *et al.*, 2014) in terms of the coordination geometry around the central metal. In this article, we report the synthesis of the title Schiff base–Pd^{II} complex and its characterization by spectroscopy and elemental analysis. The X-ray structure (Fig. 1), confirms the binding mode of the 4-fluorobenzyl(iminoethyl)phenolate ligand to the Pd^{II} cation.


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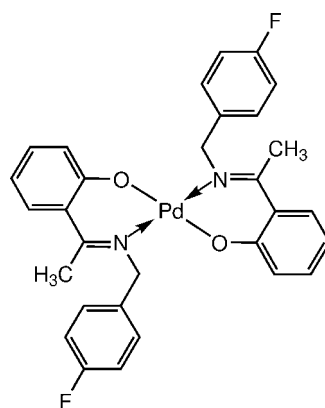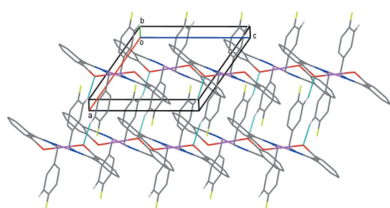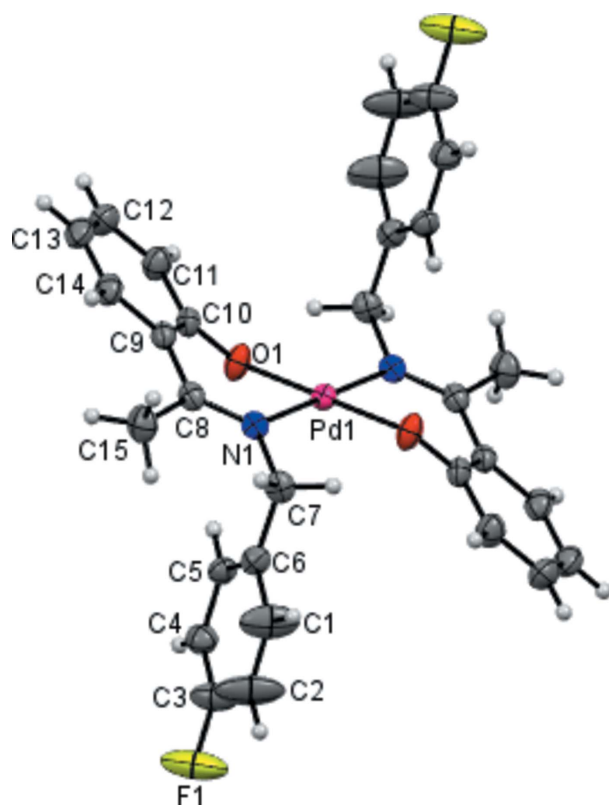
Figure 1
The molecular structure of (1), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The labelled atoms are related to the unlabelled atoms of the Schiff base ligands by the symmetry code $1 - x, 2 - y, 2 - z$.

The title compound (1) was screened for catalytic activity in the Suzuki cross-coupling reaction between phenylboronic acid and iodobenzene with a catalyst loading of 1 mmol%. The conversion of iodobenzene was found to occur with a yield of 52%.

2. Structural commentary

The asymmetric unit of (1) contains one-half of the molecule with the Pd^{II} cation lying on an inversion centre and the Schiff base anion acting as an *N,O* bidentate chelate ligand (Fig. 1).
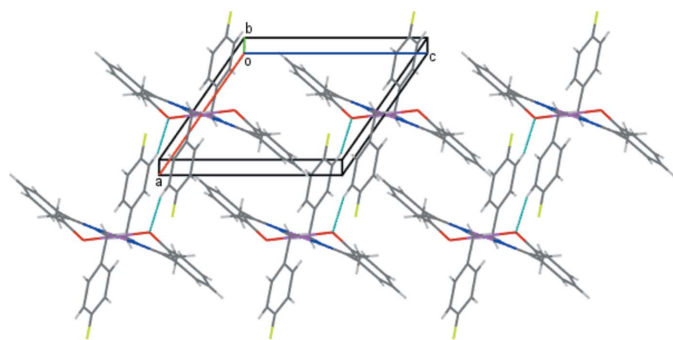
Figure 2
Screw chains of molecules of (1) linked by C—H⋯O interactions (drawn as dashed lines).

Table 1
Selected geometric parameters (Å, °).

Pd1—O1	1.9770 (18)	Pd1—N1	2.028 (2)
O1—Pd1—N1	88.48 (8)	O1^i—Pd1—N1	91.52 (8)

Symmetry code: (i) $-x + 1, -y + 2, -z + 2$.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C4—H4A⋯O1^{ii}	0.93	2.50	3.405 (5)	165

Symmetry code: (ii) $-x + 2, -y + 2, -z + 2$.

The Pd^{II} cation binds to the N and the O atoms of two symmetry-related Schiff base ligand such that the N and O atoms are mutually *trans*. The N$_2$O$_2$ donor sets of the two chelating Schiff base ligands in the equatorial plane around Pd1 adopt a slightly distorted square-planar coordination geometry. The Pd1—N1 and Pd1—O1 distances (Table 1) are typical of square-planar Pd^{II} complexes, and compare well with those observed in other closely related Pd^{II} complexes (Adrian *et al.*, 2008; Bahron *et al.*, 2014; Wan Ibrahim & Shamsuddin, 2012). The bite angle of the iminomethyl-phenolate chelate, N1—Pd1—O1 is 88.48 (8)°, which is also similar to that in a related Pd^{II} complex (Bahron *et al.*, 2014). The ring Pd1/N1/C8/C9/C10/O1 adopts an envelope conformation with Pd1 displaced by 0.270 (2) Å from the plane of the other ring atoms, and with puckering parameters $Q = 0.525$ (2) Å, $\theta = 112.8$ (3) and $\varphi = 206.9$ (3)°. Other bond lengths and angles observed in the structure are also normal. The fluorophenyl ring (C1–C6) makes a dihedral angle of 66.2 (2)° with the phenolate ring (C9–C14).

3. Supramolecular features

In the crystal packing of (1), the molecules are linked into chains along the [101] direction by weak C4—H4A⋯O1 interactions (Fig. 2, Table 2). A weak π–π stacking interaction occurs between the phenolate rings of adjacent complexes (Fig. 3), with a centroid–centroid distance, $Cg4$⋯$Cg4^{iii}$, of 4.079 (2) Å [symmetry code: (iii) = $1 - x, 2 - y, 1 - z$; $Cg4$ is the centroid of the C9–C14 ring]. These combine with the C—H⋯O contacts to generate sheets in the *ac* plane (Fig. 4). These sheets are further stacked along the *b*-axis direction.

4. Database survey

Six Pd^{II} complexes with related Schiff base N$_2$O$_2$ donor sets have been reported (Brunner *et al.*, 2000; Mehta & Vengur-lekar, 2001; Bahron *et al.*, 2011, 2014; Mohd Tajuddin *et al.*, 2012a; Tsuno *et al.*, 2013). However, only three of these Pd^{II} complexes have closely related Schiff base ligands (Bahron *et al.*, 2011; 2014; Mohd Tajuddin *et al.*, 2012a).
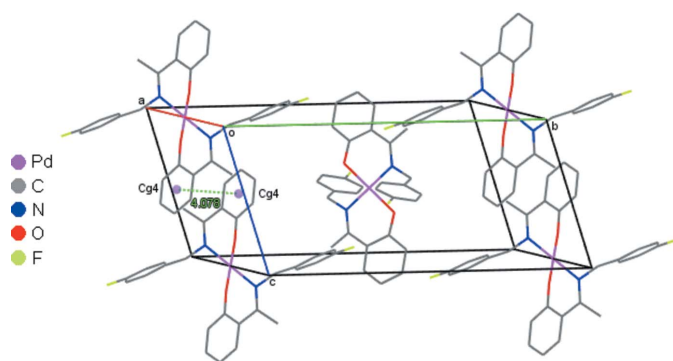
Figure 3
π–π contacts for (1) drawn as dotted lines with ring centroids shown as coloured spheres. *Cg*4 is the centroid of the C9–C14 ring. H atoms are omitted for clarity.

5. Synthesis and crystallization

The ligand, (*E*)-2-(1-(4-fluorobenzylimino)ethyl)phenol (Mohd Tajuddin *et al.*, 2012*b*) (2 mmol, 0.4877 g) was dissolved in CH$_3$CN (30 mL) in a round-bottomed flask. Palladium(II) acetate (1 mmol, 0.2251 g) was dissolved separately in CH$_3$CN (20 mL) and was then added into the flask containing the ligand solution. The mixture was stirred and refluxed for 5 h upon which a turmeric yellow solid was formed. The solid was filtered off, washed with ice-cold CH$_3$CN and air dried at room temperature. The solid product was recrystallized from chloroform, yielding yellow crystals (yield 48.5%). ^{1}H NMR, ^{13}C NMR and IR spectral bands have been studied and agree well with the structure obtained from the values of the CHN analyses and X-ray structure determination.

Melting point 508–510 K. Analytical data for C$_{30}$H$_{26}$F$_2$N$_2$O$_2$Pd: C, 60.97; H, 4.43; N, 4.74%; Found: C, 60.81; H, 4.49; N, 4.66%. IR (KBr, cm^{-1}): 1598 ν(C=N), 1319 ν(C—N), 1216 ν(C—O), 1321 ν(CH$_3$), 556 ν(Pd—N), 450 ν(Pd—O). ^{1}H NMR (300 MHz, CDCl$_3$): δ (p.p.m.) 2.32 (*s*, 3H, C—CH$_3$), 5.11 (*s*, 2H, CH$_2$), 6.53–7.46 (ArC). ^{13}C NMR (300 MHz, CDCl$_3$): δ (p.p.m.) 19.5 (C—CH$_3$), 54.2 (CH$_2$), 115.3, 115.6, 121.3, 128.6, 130.2 (ArC), 169.8 (C=N).

The infrared spectrum of (1) exhibits a strong band at 1598 cm^{-1} assignable to the C=N stretching frequency of the azomethine moiety. Weak bands at 556 and 450 cm^{-1} attributable to Pd—N and Pd—O vibrations, respectively (Ouf *et al.*, 2010), are due to the participation of the nitrogen of the azomethine group and the oxygen of the phenolate ring in the complexation of the palladium(II) centre by the Schiff base ligands. From the NMR results, the free 4-fluorobenzyl-(iminoethyl)phenolate ligand shows a multiplet at around 6.80–7.57 p.p.m. assignable to the aromatic protons. A corresponding multiplet appears in almost the same position in the spectrum of the Pd^{II} complex (compound 1) as that observed by Gupta *et al.* (2013). Singlets for aliphatic methylene (–CH$_2$) and methyl (–CH$_3$) protons appear at 5.11 and 2.32 p.p.m., respectively. The ^{13}C chemical shift for the imine carbon (C=N) is found at 169.8 p.p.m., agreeing with data reported by Şenol *et al.* (2011).

Table 3
Experimental details.

Crystal data	
Chemical formula	[Pd(C$_{15}$H$_{13}$FNO)$_2$]
M_r	590.93
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	7.5924 (5), 21.9212 (14), 9.3475 (5)
β (°)	124.963 (4)
V (Å^3)	1274.97 (15)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.77
Crystal size (mm)	0.50 × 0.25 × 0.25
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.699, 0.830
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38866, 2776, 2720
R_{int}	0.057
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.073, 1.30
No. of reflections	2776
No. of parameters	170
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.48

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

The title compound was screened for catalytic activity in the Suzuki cross-coupling reaction between phenylboronic acid with iodobenzene. The reaction was carried out under nitrogen at 373 K in dimethylacetamide with a catalyst loading of 1 mmol%. The conversion of iodobenzene was monitored using GC–FID after 24 hours of reaction time. This resulted in a 52% conversion of iodobenzene in the reaction.

6. Refinement

Crystal data, data collection and crystal structure refinement details are summarized in Table 3. All H atoms were posi-
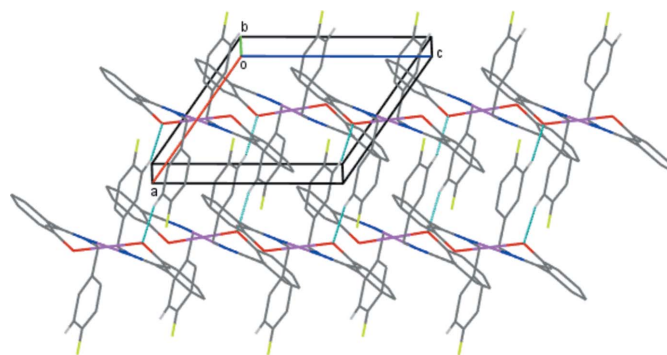
Figure 4
The packing of (1) viewed approximately along the *b* axis showing molecular sheets of the Pd^{II} complex. Only H atoms involved in C—H⋯O interactions are shown for clarity.

tioned geometrically and allowed to ride on their parent atoms, with $d(C—H) = 0.93$ Å for aromatic, 0.97 Å for CH_2 and 0.96 Å for CH_3 hydrogen atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

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Crystal structure of bis(2-{1-[(*E*)-(4-fluorobenzyl)imino]ethyl}phenolato-$\kappa^2 N,O$)palladium(II)

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Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

Bis(2-{1-[(*E*)-(4-fluorobenzyl)imino]ethyl}phenolato-$\kappa^2 N,O$)palladium(II)

Crystal data

$[\text{Pd}(\text{C}_{15}\text{H}_{13}\text{FNO})_2]$	$F(000) = 600$
$M_r = 590.93$	$D_x = 1.539$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 508–510 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.5924$ (5) Å	Cell parameters from 2776 reflections
$b = 21.9212$ (14) Å	$\theta = 3.2$–27.0°
$c = 9.3475$ (5) Å	$\mu = 0.77$ mm^{-1}
$\beta = 124.963$ (4)°	$T = 296$ K
$V = 1274.97$ (15) Å^3	Block, yellow
$Z = 2$	$0.50 \times 0.25 \times 0.25$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer	38866 measured reflections
Radiation source: sealed tube	2776 independent reflections
Graphite monochromator	2720 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.057$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$\theta_{max} = 27.0°$, $\theta_{min} = 3.2°$
$T_{min} = 0.699$, $T_{max} = 0.830$	$h = -9 \rightarrow 9$
	$k = -28 \rightarrow 28$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.034$	
$wR(F^2) = 0.073$	Secondary atom site location: difference Fourier map
$S = 1.30$	
2776 reflections	Hydrogen site location: inferred from neighbouring sites
170 parameters	

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0086P)^2 + 1.3994P]$
  where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Special details

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

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 > 2sigma(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	0.5000	1.0000	1.0000	0.03202 (9)
F1	1.3139 (4)	0.77987 (11)	1.2186 (5)	0.1153 (11)
O1	0.5384 (3)	1.04581 (9)	0.8375 (2)	0.0462 (5)
N1	0.4268 (3)	0.92521 (9)	0.8478 (3)	0.0343 (4)
C1	0.7655 (7)	0.78728 (16)	1.0865 (7)	0.0924 (16)
H1A	0.6670	0.7629	1.0890	0.111*
C2	0.9701 (7)	0.76567 (18)	1.1567 (8)	0.117 (2)
H2A	1.0108	0.7272	1.2078	0.140*
C3	1.1113 (6)	0.80149 (15)	1.1502 (6)	0.0716 (11)
C4	1.0618 (5)	0.85845 (14)	1.0834 (4)	0.0495 (7)
H4A	1.1627	0.8827	1.0839	0.059*
C5	0.8555 (5)	0.87966 (12)	1.0140 (4)	0.0416 (6)
H5	0.8184	0.9188	0.9670	0.050*
C6	0.7048 (5)	0.84467 (12)	1.0125 (4)	0.0411 (6)
C7	0.4795 (5)	0.86633 (12)	0.9399 (4)	0.0429 (6)
H7A	0.3781	0.8358	0.8598	0.051*
H7B	0.4629	0.8702	1.0349	0.051*
C8	0.3497 (4)	0.92650 (12)	0.6831 (4)	0.0382 (6)
C9	0.2963 (4)	0.98338 (13)	0.5855 (3)	0.0381 (6)
C10	0.3929 (4)	1.03958 (13)	0.6678 (3)	0.0390 (6)
C11	0.3352 (6)	1.09165 (15)	0.5625 (4)	0.0527 (7)
H11A	0.3971	1.1289	0.6147	0.063*
C12	0.1898 (6)	1.08905 (16)	0.3845 (4)	0.0578 (8)
H12A	0.1554	1.1243	0.3181	0.069*
C13	0.0945 (5)	1.03431 (17)	0.3037 (4)	0.0551 (8)
H13A	−0.0052	1.0326	0.1833	0.066*
C14	0.1479 (5)	0.98286 (15)	0.4023 (4)	0.0482 (7)
H14A	0.0844	0.9461	0.3468	0.058*
C15	0.3123 (6)	0.86788 (14)	0.5833 (4)	0.0566 (8)
H15A	0.3280	0.8756	0.4900	0.085*
H15B	0.1698	0.8531	0.5359	0.085*
H15C	0.4154	0.8378	0.6608	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.03017 (15)	0.03263 (14)	0.03135 (14)	−0.00387 (10)	0.01650 (11)	−0.00210 (11)
F1	0.0547 (14)	0.0598 (14)	0.175 (3)	0.0194 (11)	0.0329 (16)	0.0054 (16)
O1	0.0568 (12)	0.0479 (11)	0.0349 (10)	−0.0199 (9)	0.0269 (9)	−0.0048 (8)
N1	0.0332 (11)	0.0332 (10)	0.0370 (11)	−0.0041 (8)	0.0203 (9)	−0.0044 (9)
C1	0.062 (2)	0.0424 (19)	0.143 (4)	−0.0064 (17)	0.041 (3)	0.027 (2)
C2	0.066 (3)	0.042 (2)	0.183 (6)	0.0083 (19)	0.036 (3)	0.038 (3)
C3	0.0486 (19)	0.0420 (17)	0.089 (3)	0.0076 (15)	0.0185 (19)	−0.0048 (17)
C4	0.0444 (16)	0.0509 (17)	0.0489 (17)	0.0005 (13)	0.0242 (14)	−0.0016 (13)
C5	0.0495 (16)	0.0367 (13)	0.0406 (14)	0.0042 (12)	0.0269 (13)	0.0054 (11)
C6	0.0476 (15)	0.0316 (12)	0.0381 (14)	−0.0029 (11)	0.0211 (12)	−0.0027 (11)
C7	0.0504 (16)	0.0328 (13)	0.0514 (16)	−0.0084 (11)	0.0327 (14)	−0.0041 (12)
C8	0.0335 (13)	0.0426 (14)	0.0395 (14)	−0.0059 (11)	0.0215 (12)	−0.0100 (11)
C9	0.0350 (13)	0.0478 (15)	0.0337 (13)	−0.0014 (11)	0.0209 (11)	−0.0032 (11)
C10	0.0424 (14)	0.0460 (15)	0.0363 (14)	−0.0025 (12)	0.0271 (12)	−0.0016 (11)
C11	0.067 (2)	0.0483 (17)	0.0498 (18)	−0.0012 (15)	0.0373 (17)	0.0029 (13)
C12	0.065 (2)	0.062 (2)	0.0513 (18)	0.0141 (16)	0.0365 (17)	0.0169 (16)
C13	0.0447 (17)	0.079 (2)	0.0360 (15)	0.0042 (16)	0.0197 (13)	0.0037 (15)
C14	0.0422 (15)	0.0614 (18)	0.0375 (15)	−0.0046 (13)	0.0208 (13)	−0.0066 (13)
C15	0.070 (2)	0.0485 (17)	0.0523 (18)	−0.0102 (15)	0.0360 (17)	−0.0160 (14)

Geometric parameters (Å, º)

Pd1—O1	1.9770 (18)	C6—C7	1.510 (4)
Pd1—O1^i	1.9770 (18)	C7—H7A	0.9700
Pd1—N1^i	2.028 (2)	C7—H7B	0.9700
Pd1—N1	2.028 (2)	C8—C9	1.458 (4)
F1—C3	1.369 (4)	C8—C15	1.516 (4)
O1—C10	1.321 (3)	C9—C14	1.411 (4)
N1—C8	1.297 (3)	C9—C10	1.415 (4)
N1—C7	1.474 (3)	C10—C11	1.403 (4)
C1—C2	1.378 (6)	C11—C12	1.373 (5)
C1—C6	1.381 (4)	C11—H11A	0.9300
C1—H1A	0.9300	C12—C13	1.381 (5)
C2—C3	1.358 (6)	C12—H12A	0.9300
C2—H2A	0.9300	C13—C14	1.363 (5)
C3—C4	1.349 (5)	C13—H13A	0.9300
C4—C5	1.387 (4)	C14—H14A	0.9300
C4—H4A	0.9300	C15—H15A	0.9600
C5—C6	1.371 (4)	C15—H15B	0.9600
C5—H5	0.9300	C15—H15C	0.9600
O1—Pd1—O1^i	180.00 (10)	N1—C7—H7B	108.9
O1—Pd1—N1^i	91.52 (8)	C6—C7—H7B	108.9
O1^i—Pd1—N1^i	88.48 (8)	H7A—C7—H7B	107.7
O1—Pd1—N1	88.48 (8)	N1—C8—C9	122.4 (2)

O1ⁱ—Pd1—N1	91.52 (8)	N1—C8—C15	120.7 (3)
N1ⁱ—Pd1—N1	180.000 (1)	C9—C8—C15	116.9 (2)
C10—O1—Pd1	118.68 (16)	C14—C9—C10	118.1 (3)
C8—N1—C7	120.0 (2)	C14—C9—C8	119.6 (3)
C8—N1—Pd1	124.82 (18)	C10—C9—C8	122.2 (2)
C7—N1—Pd1	115.13 (17)	O1—C10—C11	117.9 (3)
C2—C1—C6	120.9 (4)	O1—C10—C9	124.0 (2)
C2—C1—H1A	119.6	C11—C10—C9	118.1 (3)
C6—C1—H1A	119.6	C12—C11—C10	121.8 (3)
C3—C2—C1	118.9 (4)	C12—C11—H11A	119.1
C3—C2—H2A	120.6	C10—C11—H11A	119.1
C1—C2—H2A	120.6	C11—C12—C13	120.3 (3)
C4—C3—C2	122.6 (3)	C11—C12—H12A	119.9
C4—C3—F1	118.5 (4)	C13—C12—H12A	119.9
C2—C3—F1	118.9 (3)	C14—C13—C12	119.3 (3)
C3—C4—C5	117.8 (3)	C14—C13—H13A	120.3
C3—C4—H4A	121.1	C12—C13—H13A	120.3
C5—C4—H4A	121.1	C13—C14—C9	122.4 (3)
C6—C5—C4	121.9 (3)	C13—C14—H14A	118.8
C6—C5—H5	119.0	C9—C14—H14A	118.8
C4—C5—H5	119.0	C8—C15—H15A	109.5
C5—C6—C1	117.9 (3)	C8—C15—H15B	109.5
C5—C6—C7	123.5 (2)	H15A—C15—H15B	109.5
C1—C6—C7	118.6 (3)	C8—C15—H15C	109.5
N1—C7—C6	113.4 (2)	H15A—C15—H15C	109.5
N1—C7—H7A	108.9	H15B—C15—H15C	109.5
C6—C7—H7A	108.9		
N1ⁱ—Pd1—O1—C10	−134.7 (2)	Pd1—N1—C8—C9	−3.2 (4)
N1—Pd1—O1—C10	45.3 (2)	C7—N1—C8—C15	0.2 (4)
O1—Pd1—N1—C8	−25.1 (2)	Pd1—N1—C8—C15	176.5 (2)
O1ⁱ—Pd1—N1—C8	154.9 (2)	N1—C8—C9—C14	−157.8 (3)
O1—Pd1—N1—C7	151.39 (18)	C15—C8—C9—C14	22.6 (4)
O1ⁱ—Pd1—N1—C7	−28.61 (18)	N1—C8—C9—C10	24.0 (4)
C6—C1—C2—C3	−0.8 (9)	C15—C8—C9—C10	−155.6 (3)
C1—C2—C3—C4	2.6 (9)	Pd1—O1—C10—C11	141.1 (2)
C1—C2—C3—F1	−179.5 (5)	Pd1—O1—C10—C9	−40.7 (3)
C2—C3—C4—C5	−2.3 (7)	C14—C9—C10—O1	−178.0 (3)
F1—C3—C4—C5	179.8 (3)	C8—C9—C10—O1	0.2 (4)
C3—C4—C5—C6	0.2 (5)	C14—C9—C10—C11	0.2 (4)
C4—C5—C6—C1	1.4 (5)	C8—C9—C10—C11	178.4 (3)
C4—C5—C6—C7	179.4 (3)	O1—C10—C11—C12	178.2 (3)
C2—C1—C6—C5	−1.1 (7)	C9—C10—C11—C12	−0.2 (5)
C2—C1—C6—C7	−179.1 (5)	C10—C11—C12—C13	0.4 (5)
C8—N1—C7—C6	87.6 (3)	C11—C12—C13—C14	−0.7 (5)
Pd1—N1—C7—C6	−89.0 (2)	C12—C13—C14—C9	0.8 (5)
C5—C6—C7—N1	8.3 (4)	C10—C9—C14—C13	−0.6 (4)

| C1—C6—C7—N1 | −173.7 (3) | C8—C9—C14—C13 | −178.8 (3) |
| C7—N1—C8—C9 | −179.5 (2) | | |

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1ⁱⁱ	0.93	2.50	3.405 (5)	165

Symmetry code: (ii) −*x*+2, −*y*+2, −*z*+2.