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Bis{2-methoxy-6-[(*E*)-(4-methylbenzyl)-iminomethyl]phenolato}palladium(II) chloroform monosolvate

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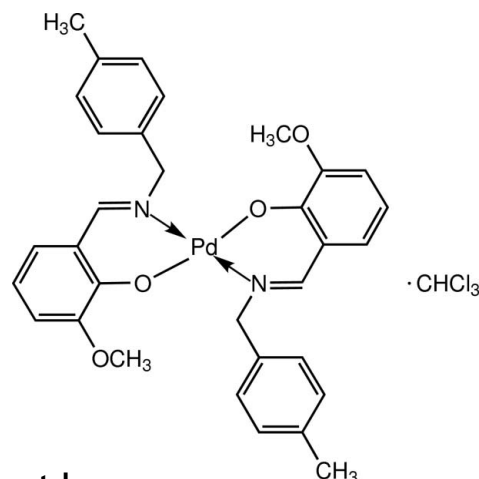
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in solvent or counterion; R factor = 0.029; wR factor = 0.073; data-to-parameter ratio = 27.2.

In the title complex, $[\text{Pd}(\text{C}_{16}\text{H}_{16}\text{NO}_2)_2] \cdot \text{CHCl}_3$, the Pd^{II} cation lies on an inversion center. One Cl atom of the CHCl_3 solvent molecule lies on a twofold axis and the C—H group is disordered with equal occupancies about this axis with the other Cl atom in a general position with full occupancy. The Pd^{II} cation is four-coordinate and adopts a square-planar geometry *via* coordination of the imine N and phenolic O atoms of the two bidentate Schiff base anions. The N and O atoms of these ligands are mutually *trans*. The plane of the benzene ring makes a dihedral angle of $73.52(10)^\circ$ with that of the methoxyphenolate ring. In the crystal, molecules of the Pd^{II} complex are arranged into sheets parallel to the *ac* plane, and the chloroform solvent molecules are located in the interstitial areas between the complex molecules. Weak intermolecular C—H \cdots O and C—H $\cdots\pi$ interactions stabilize the packing.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related structures, see: Bahron *et al.* (2011a,b); Halder *et al.* (2008). For background to and applications of Pd^{II} complexes, see: Bowes *et al.* (2011); Geeta *et al.* (2010); Gupta & Sutar (2008); Kalita *et al.* (2014); Mohd Tajuddin *et al.* (2012); Tamizh & Karvembu (2012).



Experimental

Crystal data

$[\text{Pd}(\text{C}_{16}\text{H}_{16}\text{NO}_2)_2] \cdot \text{CHCl}_3$
 $M_r = 734.36$
Monoclinic, $C2/c$
 $a = 31.9861(8)$ Å
 $b = 5.9668(2)$ Å
 $c = 22.6135(5)$ Å
 $\beta = 134.885(1)^\circ$
 $V = 3057.92(15)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.91$ mm⁻¹
 $T = 100$ K
 $0.48 \times 0.25 \times 0.18$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.669$, $T_{\max} = 0.853$
43800 measured reflections
5542 independent reflections
5006 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.073$
 $S = 1.05$
5542 reflections
204 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 1.24$ e Å⁻³
 $\Delta\rho_{\min} = -1.90$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C9–C14 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8A \cdots O1 ⁱ	0.97	2.19	2.806 (2)	120
C14—H14A \cdots O1 ⁱ	0.93	2.57	3.284 (2)	134
C17—H17A \cdots Cg1 ⁱ	0.96	2.83	3.648 (5)	144

Symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

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

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§ Thomson Reuters ResearcherID: A-3561-2009.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5416).

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supporting information

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Bis{2-methoxy-6-[(*E*)-(4-methylbenzyl)iminomethyl]phenolato}palladium(II) chloroform monosolvate

Hadariah Bahron, Amalina Mohd Tajuddin, Wan Nazihah Wan Ibrahim, Suchada Chantrapromma and Hoong-Kun Fun

S1. Comment

Complexes of palladium(II) and nickel(II) have broad and diversified applications involving numerous fields of catalysis such as the Heck reaction, Suzuki-Miyaura coupling reactions and including also the polymerization of ethylene, epoxidation and allylic alkylation (Bowes *et al.*, 2011; Gupta & Sutar, 2008; Mohd Tajuddin *et al.*, 2012; Tamizh & Karvembu, 2012). They are also important in various aspects of bioinorganic chemistry (Geeta *et al.*, 2010; Kalita *et al.*, 2014;). The properties of such complexes depend on the coordination environment around the metal center. Schiff bases containing iminoalkylphenolato groups commonly adopt a bidentate coordination mode with metal centres as for example in bis{2-[(*E*)-(4-fluorobenzyl)iminomethyl]-6-methoxy-phenolato-*K*²*N,O*¹}nickel(II) (Bahron *et al.*, 2011*b*). In the title complex (I), [Pd(C₃₂H₃₂N₂O₄)]·(CHCl₃), the Schiff base ligand is bis-bidentate (see Fig. 1) and is related to the previously reported bis(2-(1-benzyliminoethyl)phenolato)palladium(II) (Bahron *et al.*, 2011*a*) but with different substituents on the iminoalkylphenolato and benzyl ring systems. Herein the crystal structure of (I) is reported.

The asymmetric unit of (I) consists of one half each of the complex molecule and the chloroform solvate molecule. The Pd^{II} atom lies on an inversion center while the Cl1 atom of the CHCl₃ solvate lies on a two-fold axis. The C17–H17A group is disordered with equal occupancies about this axis with Cl2 in a general position with full occupancy. These two symmetry elements generate the other halves of the Schiff base ligand and the chloroform molecule. The Pd^{II} ion is four-coordinate and adopts a square planar geometry *via* coordination to the two imine N (N1 and N1ⁱ symmetry code; *i* = 1/2 - *x*, 3/2 - *y*, 1 - *z*) and two phenolic O (O1 and O1ⁱ symmetry code; *i* = 1/2 - *x*, 3/2 - *y*, 1 - *z*) atoms of the two bidentate Schiff base anions. The imine N atoms and phenolic O atoms are in mutually *trans* positions. The Pd–N and Pd–O distances in the N₂O₂ coordination [1.9741 (10) Å and 2.0204 (12) Å, respectively] are in the same ranges as those observed in the other closely related Pd^{II} complexes of N₂O₂ Schiff base ligands (Bahron *et al.*, 2011*a* and Halder *et al.*, 2008). Other bond lengths and angles observed in the structure are also normal (Allen *et al.*, 1987). The bond angles O–Pd–N [O1–Pd1–N1 = 92.17 (5)° and O1–Pd1–N1ⁱ = 87.83 (5)° symmetry code; *i* = 1/2 - *x*, 3/2 - *y*, 1 - *z*] are close to 90°. Moreover the coordination of the two NO bidentate chelate ligands to the Pd^{II} ion results in the formation of two six-membered rings (Pd1/N1/C7/C8/C1/O1 and Pd1/N1ⁱ/C7ⁱ/C8ⁱ/C1ⁱ/O1ⁱ). The methoxy substituent deviates only slightly from the plane of the ring to which it is bound with the torsion angle C15–O2–C2–C3 = 7.9 (2)°. The benzene ring (C9–C14) makes a dihedral angle of 73.52 (10)° with the methoxyphenolate ring.

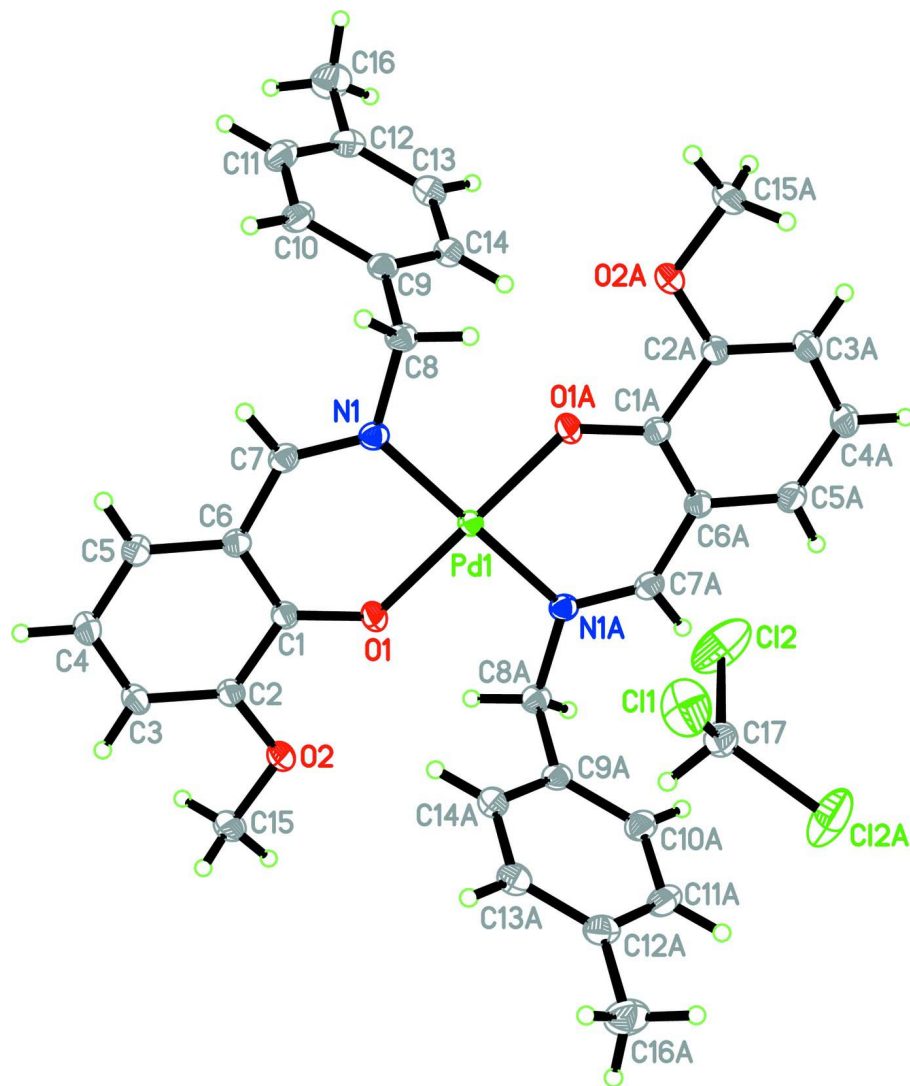
In the crystal packing (Fig. 2), molecules of the Pd^{II} complex are arranged into sheets parallel to the *ac* plane, and the chloroform solvent molecules are located in the interstitial areas between the complex molecules. Weak intermolecular C—H⋯O interactions stabilise the packing. A C—H⋯π interaction involving the centroid of the (C9–C14) benzene ring, Cg₁, is also observed, (Table 1).

S2. Experimental

The ligand, (*E*)-2-methoxy-6-((4-methylbenzylimino)methyl)-phenol (5 mmol, 1.2765 g) was dissolved in CH₃CN (10 ml) in a round-bottomed flask. Palladium(II) acetate (2.5 mmol, 0.5612 g) was dissolved separately in CH₃CN (10 ml) and added to the flask containing the ligand solution. The mixture was refluxed with stirring for 4 h upon which a dark yellow solid was formed. The solid was filtered off, washed with ice-cold CH₃CN and air dried at room temperature. The solid product was recrystallized from CHCl₃ yielding orange crystals. Yield 94.4%. Melting point 236–238 °C. ¹H NMR (300 MHz, CDCl₃, p.p.m.): δ = 2.30 (s, 3H, CH₃), 5.07 (s, 2H, CH₂), 3.75 (s, 3H, Ar-OCH₃), 6.76–7.34 (m, 7H, ArH), 7.69 (s, 1H, =CH). ¹³C NMR (300 MHz, CDCl₃): 21.1 (CH₃), 55.9 (Ar-OCH₃), 62.25 (CH₂), 114.0, 120.4, 125.4, 128.4, 129.1, 136.1 (ArC), 162.6 (N=CH). Analytical calculation for C₃₂H₃₂N₂O₄Pd: C, 62.49; H, 5.24; N, 4.55; Found: C, 62.47; H, 5.29; N, 4.55. IR (KBr, cm⁻¹): ν (C=N) 1623 (s), ν (C—N) 1316 (s), ν (C—O) 1239 (s), ν (OCH₃) 1092 (w), ν (Pd—O) 660 (w), ν (Pd—N) 416 (w).

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with $d(\text{C—H}) = 0.93 \text{ \AA}$ for aromatic, 0.97 \AA for CH and CH₂ and 0.96 \AA for CH₃ atoms. The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.18 \AA from Cl2 and the deepest hole is located at 0.71 \AA from Cl2.

**Figure 1**

The molecular structure of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. Atoms with suffix A of the Schiff base ligand were generated by symmetry code: $1/2 - x, 3/2 - y, 1 - z$. Only one disorder component of the disordered C–H group of the chloroform solvate is shown for clarity, and C12A atom was generated by symmetry code: $-x, y, 1/2 - z$.

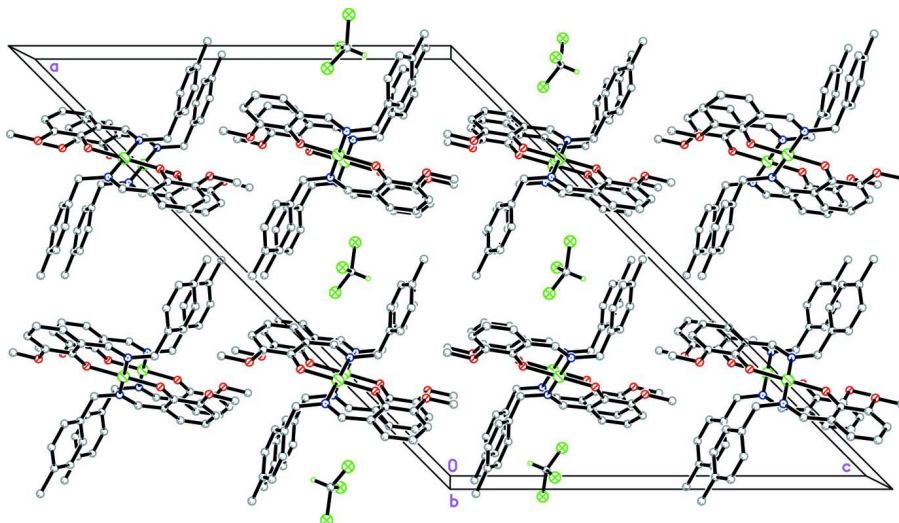


Figure 2

The crystal packing of (I) viewed along the *b* axis showing the stacking of molecules of the Pd^{II} complex. H atoms were omitted and only one disorder component of the disordered C–H group of the chloroform solvate is shown for clarity.

Bis{2-methoxy-6-[(*E*)-(4-methylbenzyl)iminomethyl]phenolato}palladium(II) chloroform monosolvate

Crystal data

[Pd(C₁₆H₁₆NO)₂]·CHCl₃

M_r = 734.36

Monoclinic, *C2/c*

Hall symbol: -*C* 2yc

a = 31.9861 (8) Å

b = 5.9668 (2) Å

c = 22.6135 (5) Å

β = 134.885 (1)°

V = 3057.92 (15) Å³

Z = 4

F(000) = 1496

D_x = 1.595 Mg m⁻³

Melting point = 509–511 K

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 5542 reflections

θ = 1.8–32.5°

μ = 0.91 mm⁻¹

T = 100 K

Block, orange

0.48 × 0.25 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

T_{min} = 0.669, *T_{max}* = 0.853

43800 measured reflections

5542 independent reflections

5006 reflections with *I* > 2σ(*I*)

R_{int} = 0.021

θ_{\max} = 32.5°, θ_{\min} = 1.8°

h = -48→48

k = -9→8

l = -33→34

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.029

wR(*F*²) = 0.073

S = 1.05

5542 reflections

204 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 8.064P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.24 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.90 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pd1	0.2500	0.7500	0.5000	0.01355 (4)	
O1	0.27424 (5)	0.77360 (19)	0.44058 (7)	0.0199 (2)	
O2	0.29036 (5)	0.7333 (2)	0.34385 (7)	0.0216 (2)	
N1	0.29650 (5)	1.0260 (2)	0.56892 (7)	0.0161 (2)	
C1	0.30562 (6)	0.9327 (2)	0.44764 (8)	0.0163 (2)	
C2	0.31517 (6)	0.9175 (3)	0.39460 (9)	0.0182 (2)	
C3	0.34628 (7)	1.0811 (3)	0.39600 (9)	0.0230 (3)	
H3A	0.3517	1.0693	0.3607	0.028*	
C4	0.36987 (8)	1.2650 (3)	0.44999 (10)	0.0256 (3)	
H4A	0.3909	1.3743	0.4505	0.031*	
C5	0.36196 (7)	1.2838 (3)	0.50202 (10)	0.0229 (3)	
H5A	0.3777	1.4061	0.5378	0.028*	
C6	0.32999 (6)	1.1187 (2)	0.50177 (8)	0.0172 (2)	
C7	0.32398 (6)	1.1514 (2)	0.55844 (9)	0.0176 (2)	
H7A	0.3421	1.2786	0.5918	0.021*	
C8	0.30159 (6)	1.0981 (3)	0.63693 (9)	0.0180 (2)	
H8A	0.2676	1.0451	0.6249	0.022*	
H8B	0.3020	1.2605	0.6393	0.022*	
C9	0.35728 (6)	1.0068 (2)	0.72040 (9)	0.0169 (2)	
C10	0.40868 (7)	1.1352 (3)	0.77237 (9)	0.0215 (3)	
H10A	0.4083	1.2778	0.7555	0.026*	
C11	0.46054 (7)	1.0533 (3)	0.84920 (10)	0.0245 (3)	
H11A	0.4943	1.1418	0.8829	0.029*	
C12	0.46238 (7)	0.8403 (3)	0.87610 (9)	0.0220 (3)	
C13	0.41100 (7)	0.7121 (3)	0.82397 (10)	0.0213 (3)	
H13A	0.4114	0.5695	0.8409	0.026*	
C14	0.35894 (7)	0.7929 (3)	0.74686 (9)	0.0197 (3)	
H14A	0.3253	0.7038	0.7130	0.024*	
C15	0.30447 (7)	0.6982 (3)	0.29710 (10)	0.0257 (3)	
H15A	0.2903	0.5538	0.2708	0.039*	

H15B	0.3465	0.7047	0.3339	0.039*	
H15C	0.2861	0.8125	0.2552	0.039*	
C16	0.51830 (8)	0.7502 (3)	0.95912 (11)	0.0325 (4)	
H16A	0.5514	0.7914	0.9680	0.049*	
H16B	0.5160	0.5899	0.9593	0.049*	
H16C	0.5232	0.8119	1.0029	0.049*	
C17	0.00983 (14)	0.8371 (6)	0.2433 (2)	0.0230 (6)	0.50
H17A	0.0259	0.8362	0.2200	0.028*	0.50
Cl1	0.0000	1.12294 (11)	0.2500	0.04186 (16)	
Cl2	0.05936 (2)	0.70272 (10)	0.33308 (4)	0.04878 (16)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01277 (6)	0.01580 (7)	0.01323 (7)	-0.00043 (4)	0.00959 (6)	-0.00051 (4)
O1	0.0230 (5)	0.0231 (5)	0.0223 (5)	-0.0064 (4)	0.0191 (5)	-0.0050 (4)
O2	0.0230 (5)	0.0280 (6)	0.0217 (5)	-0.0055 (4)	0.0185 (5)	-0.0047 (4)
N1	0.0145 (5)	0.0181 (5)	0.0143 (5)	0.0009 (4)	0.0097 (4)	-0.0003 (4)
C1	0.0133 (5)	0.0203 (6)	0.0138 (5)	0.0002 (4)	0.0090 (5)	0.0020 (4)
C2	0.0144 (5)	0.0243 (7)	0.0141 (5)	-0.0012 (5)	0.0095 (5)	0.0014 (5)
C3	0.0205 (6)	0.0314 (8)	0.0182 (6)	-0.0042 (6)	0.0141 (6)	0.0022 (6)
C4	0.0247 (7)	0.0297 (8)	0.0210 (7)	-0.0081 (6)	0.0156 (6)	0.0016 (6)
C5	0.0213 (7)	0.0251 (7)	0.0179 (6)	-0.0064 (5)	0.0122 (6)	-0.0005 (5)
C6	0.0144 (5)	0.0200 (6)	0.0132 (5)	-0.0006 (5)	0.0083 (5)	0.0019 (5)
C7	0.0152 (5)	0.0179 (6)	0.0147 (5)	-0.0001 (5)	0.0088 (5)	0.0001 (4)
C8	0.0182 (6)	0.0192 (6)	0.0181 (6)	0.0007 (5)	0.0134 (5)	-0.0023 (5)
C9	0.0177 (6)	0.0191 (6)	0.0159 (5)	-0.0001 (5)	0.0126 (5)	-0.0029 (5)
C10	0.0219 (6)	0.0203 (6)	0.0191 (6)	-0.0032 (5)	0.0134 (6)	-0.0033 (5)
C11	0.0206 (6)	0.0264 (7)	0.0186 (6)	-0.0046 (6)	0.0111 (6)	-0.0043 (5)
C12	0.0207 (6)	0.0271 (7)	0.0173 (6)	0.0025 (5)	0.0131 (6)	-0.0005 (5)
C13	0.0235 (7)	0.0220 (6)	0.0213 (6)	0.0017 (5)	0.0168 (6)	0.0008 (5)
C14	0.0197 (6)	0.0223 (6)	0.0192 (6)	-0.0014 (5)	0.0145 (6)	-0.0016 (5)
C15	0.0249 (7)	0.0374 (9)	0.0234 (7)	-0.0029 (6)	0.0202 (6)	-0.0036 (6)
C16	0.0251 (8)	0.0385 (10)	0.0215 (7)	0.0054 (7)	0.0120 (7)	0.0050 (7)
C17	0.0241 (14)	0.0232 (14)	0.0245 (14)	-0.0037 (11)	0.0181 (12)	-0.0041 (11)
Cl1	0.0565 (4)	0.0199 (3)	0.0593 (5)	0.000	0.0445 (4)	0.000
Cl2	0.0256 (2)	0.0353 (2)	0.0438 (3)	0.00892 (18)	0.0097 (2)	-0.0081 (2)

Geometric parameters (Å, °)

Pd1—O1 ⁱ	1.9741 (10)	C9—C14	1.395 (2)
Pd1—O1	1.9741 (10)	C10—C11	1.393 (2)
Pd1—N1	2.0204 (12)	C10—H10A	0.9300
Pd1—N1 ⁱ	2.0204 (12)	C11—C12	1.392 (2)
O1—C1	1.3069 (17)	C11—H11A	0.9300
O2—C2	1.3672 (19)	C12—C13	1.393 (2)
O2—C15	1.4279 (18)	C12—C16	1.508 (2)
N1—C7	1.2971 (19)	C13—C14	1.396 (2)

N1—C8	1.4911 (18)	C13—H13A	0.9300
C1—C6	1.411 (2)	C14—H14A	0.9300
C1—C2	1.4344 (19)	C15—H15A	0.9600
C2—C3	1.378 (2)	C15—H15B	0.9600
C3—C4	1.401 (2)	C15—H15C	0.9600
C3—H3A	0.9300	C16—H16A	0.9600
C4—C5	1.372 (2)	C16—H16B	0.9600
C4—H4A	0.9300	C16—H16C	0.9600
C5—C6	1.417 (2)	C17—C17 ⁱⁱ	0.871 (6)
C5—H5A	0.9300	C17—C12	1.654 (3)
C6—C7	1.437 (2)	C17—C11	1.760 (3)
C7—H7A	0.9300	C17—C12 ⁱⁱ	1.769 (3)
C8—C9	1.512 (2)	C17—H17A	0.9604
C8—H8A	0.9700	C11—C17 ⁱⁱ	1.760 (3)
C8—H8B	0.9700	C12—C17 ⁱⁱ	1.769 (3)
C9—C10	1.394 (2)		
O1 ⁱ —Pd1—O1	180.000 (1)	C10—C9—C8	120.25 (14)
O1 ⁱ —Pd1—N1	87.83 (5)	C14—C9—C8	121.32 (13)
O1—Pd1—N1	92.17 (5)	C11—C10—C9	121.09 (15)
O1 ⁱ —Pd1—N1 ⁱ	92.17 (5)	C11—C10—H10A	119.5
O1—Pd1—N1 ⁱ	87.83 (5)	C9—C10—H10A	119.5
N1—Pd1—N1 ⁱ	180.0	C12—C11—C10	120.73 (15)
C1—O1—Pd1	127.25 (9)	C12—C11—H11A	119.6
C2—O2—C15	116.10 (12)	C10—C11—H11A	119.6
C7—N1—C8	115.30 (12)	C11—C12—C13	118.08 (14)
C7—N1—Pd1	123.66 (10)	C11—C12—C16	121.11 (16)
C8—N1—Pd1	121.04 (9)	C13—C12—C16	120.82 (16)
O1—C1—C6	125.72 (13)	C12—C13—C14	121.50 (15)
O1—C1—C2	116.75 (13)	C12—C13—H13A	119.2
C6—C1—C2	117.52 (13)	C14—C13—H13A	119.2
O2—C2—C3	124.80 (13)	C9—C14—C13	120.18 (14)
O2—C2—C1	114.39 (12)	C9—C14—H14A	119.9
C3—C2—C1	120.81 (14)	C13—C14—H14A	119.9
C2—C3—C4	120.72 (14)	O2—C15—H15A	109.5
C2—C3—H3A	119.6	O2—C15—H15B	109.5
C4—C3—H3A	119.6	H15A—C15—H15B	109.5
C5—C4—C3	119.97 (15)	O2—C15—H15C	109.5
C5—C4—H4A	120.0	H15A—C15—H15C	109.5
C3—C4—H4A	120.0	H15B—C15—H15C	109.5
C4—C5—C6	120.60 (15)	C12—C16—H16A	109.5
C4—C5—H5A	119.7	C12—C16—H16B	109.5
C6—C5—H5A	119.7	H16A—C16—H16B	109.5
C1—C6—C5	120.37 (13)	C12—C16—H16C	109.5
C1—C6—C7	122.75 (13)	H16A—C16—H16C	109.5
C5—C6—C7	116.89 (14)	H16B—C16—H16C	109.5
N1—C7—C6	128.23 (14)	C17 ⁱⁱ —C17—C12	82.7 (4)
N1—C7—H7A	115.9	C17 ⁱⁱ —C17—C11	75.67 (10)

C6—C7—H7A	115.9	C12—C17—C11	115.99 (18)
N1—C8—C9	111.02 (11)	C17 ⁱⁱ —C17—C12 ⁱⁱ	68.1 (4)
N1—C8—H8A	109.4	C12—C17—C12 ⁱⁱ	115.65 (19)
C9—C8—H8A	109.4	C11—C17—C12 ⁱⁱ	110.29 (18)
N1—C8—H8B	109.4	C17 ⁱⁱ —C17—H17A	171.5
C9—C8—H8B	109.4	C12—C17—H17A	104.5
H8A—C8—H8B	108.0	C11—C17—H17A	104.5
C10—C9—C14	118.42 (14)	C12 ⁱⁱ —C17—H17A	104.4
N1—Pd1—O1—C1	-4.24 (13)	C4—C5—C6—C7	179.83 (15)
N1 ⁱ —Pd1—O1—C1	175.76 (13)	C8—N1—C7—C6	176.22 (13)
O1 ⁱ —Pd1—N1—C7	-175.14 (12)	Pd1—N1—C7—C6	-3.4 (2)
O1—Pd1—N1—C7	4.86 (12)	C1—C6—C7—N1	-0.7 (2)
O1 ⁱ —Pd1—N1—C8	5.26 (10)	C5—C6—C7—N1	179.23 (15)
O1—Pd1—N1—C8	-174.74 (10)	C7—N1—C8—C9	-85.20 (15)
Pd1—O1—C1—C6	1.8 (2)	Pd1—N1—C8—C9	94.43 (13)
Pd1—O1—C1—C2	-177.17 (10)	N1—C8—C9—C10	93.72 (16)
C15—O2—C2—C3	7.9 (2)	N1—C8—C9—C14	-85.35 (16)
C15—O2—C2—C1	-173.07 (13)	C14—C9—C10—C11	-0.4 (2)
O1—C1—C2—O2	-0.92 (19)	C8—C9—C10—C11	-179.47 (14)
C6—C1—C2—O2	180.00 (12)	C9—C10—C11—C12	0.1 (2)
O1—C1—C2—C3	178.12 (14)	C10—C11—C12—C13	0.1 (2)
C6—C1—C2—C3	-1.0 (2)	C10—C11—C12—C16	179.97 (16)
O2—C2—C3—C4	179.63 (15)	C11—C12—C13—C14	0.0 (2)
C1—C2—C3—C4	0.7 (2)	C16—C12—C13—C14	-179.83 (15)
C2—C3—C4—C5	-0.2 (3)	C10—C9—C14—C13	0.5 (2)
C3—C4—C5—C6	-0.1 (3)	C8—C9—C14—C13	179.60 (13)
O1—C1—C6—C5	-178.26 (14)	C12—C13—C14—C9	-0.3 (2)
C2—C1—C6—C5	0.7 (2)	C12—C17—C11—C17 ⁱⁱ	-74.3 (4)
O1—C1—C6—C7	1.7 (2)	C12 ⁱⁱ —C17—C11—C17 ⁱⁱ	59.6 (4)
C2—C1—C6—C7	-179.34 (13)	C11—C17—C12—C17 ⁱⁱ	70.1 (2)
C4—C5—C6—C1	-0.2 (2)	C12 ⁱⁱ —C17—C12—C17 ⁱⁱ	-61.4 (3)

Symmetry codes: (i) $-x+1/2, -y+3/2, -z+1$; (ii) $-x, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

*Cg*1 is the centroid of the C9—C14 ring.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C8—H8A \cdots O1 ⁱ	0.97	2.19	2.806 (2)	120
C14—H14A \cdots O1 ⁱ	0.93	2.57	3.284 (2)	134
C17—H17A \cdots <i>Cg</i> 1 ⁱ	0.96	2.83	3.648 (5)	144

Symmetry code: (i) $-x+1/2, -y+3/2, -z+1$.