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trans-Dichloridobis[(*S*)-(−)-1-(4-methylphenyl)-ethylamine-κN]palladium(II)

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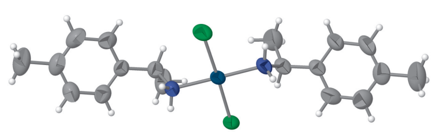
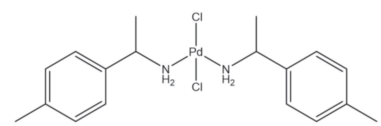
The title complex, $[PdCl_2(C_9H_{13}N)_2]$, comprises a single molecule in the asymmetric unit. The Pd^{II} atom is tetracoordinated by two N atoms from two *trans*-aligned organic ligands and two Cl ligands, forming a square-planar metal coordination environment. The distances from the *ortho*-H atoms on the phenyl ring to the central Pd^{II} atom fall within the range 4.70–5.30 Å, precluding any significant intramolecular Pd···H interactions.

3D view



Chemical scheme



Structure description

The chemistry of Pd^{II} compounds with diverse ligands represents a rich area within organometallic chemistry, extensively explored in organic synthesis (Hartwig, 1998; Müller & Beller, 1998). Pd^{II} compounds also exhibit cytotoxic activity, which makes them interesting for certain therapeutic applications. Moreover, Pd^{II} compounds with amine ligands have a central role in catalytic conversions due to the hydrogen bond developed between the amino group and the catalyst. In the presence of excess amine, 16-electron $PdCl_2L_2$ (L = amine) adducts, usually existing as a mixture of *cis* and *trans* isomers, emerge as viable starting materials for cyclopalladations (Ryabov, 1990; Cattalini & Martelli, 1969). While monodentate Pd^{II}–amine complexes tend to display general instability as reaction intermediates, bis(amine)–Pd^{II} complexes have garnered substantial attention for their involvement as intermediates in amination reactions (Widenhoefer & Buchwald, 1996; Seligson & Trogler, 1991). In this context, our focus has shifted towards complexes derived from optically pure chiral amines. We present here the molecular and crystal structures of *trans*-dichlorido bis[(*S*)-(−)-1-[(4-methylphenyl)-ethylamine]palladium(II).

The asymmetric unit comprises a single molecule, as shown in Fig. 1. The molecular complex adopts a square-planar metal coordination environment around the central Pd^{II}

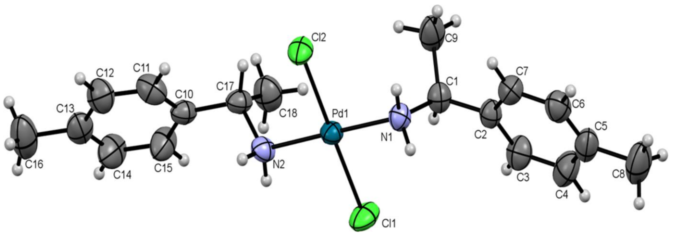


Figure 1
The molecular structure of the title complex with displacement ellipsoids drawn at the 50% probability level.

atom. There are slight distortions from the ideal square-planar geometry, as revealed by a deviation of 0.025 Å of the Pd^{II} atom from the plane defined by atoms Cl2, N2, Cl1, N1. The interatomic distances from the central Pd^{II} atom to the ligand atoms are 2.039 (4) Å [Pd1—N1] and 2.053 (4) Å [Pd1—N2]; the average Pd—Cl bond length is 2.298 Å. The pairs of Cl and amine ligands are *trans*-aligned around the central Pd^{II} atom and characterized by a Cl1—Pd1—Cl2 angle of 177.22 (6)° and an N1—Pd1—N2 angle of 179.39 (18)°; the Cl1—Pd1—N1 angle amounts to 88.25 (12)°, with other angles approximately 90°. The sp^3 hybridization of the N atoms and the C9 and C17 atoms cause the non-planarity of the molecular structure. The amine ligands are arranged differently around the central Pd^{II} atom. The Cl1—Pd1—N1—C1 torsion angle is 73.2 (3)°, compared to 53.5 (3)° for Cl2—Pd1—N2—C17. Both amine ligands exhibit a *gauche* conformation, as revealed by the torsion angle C17—N2—N1—C1 = −55.6 (4)°.

A view of the crystal packing shows that individual molecules are organized into supramolecular ribbons defined by C—H⋯Cl and N—H⋯Cl hydrogen bonding interactions (Table 1); the ribbons extend parallel to [100] (Fig. 2). The cohesion between the ribbons is accomplished mainly by weak

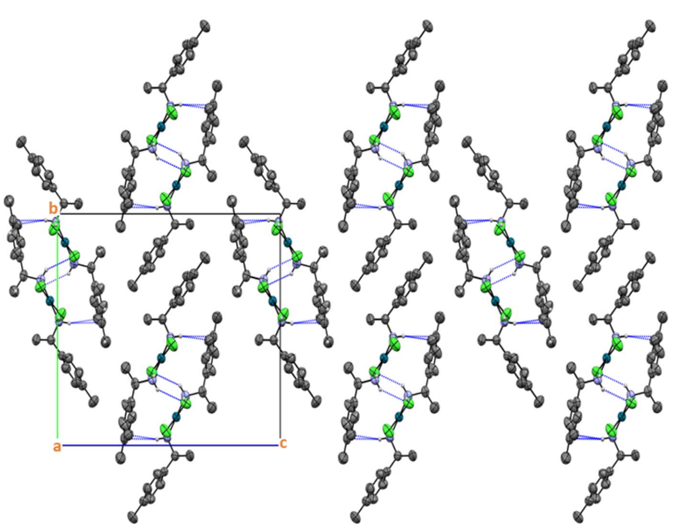


Figure 2
The crystal packing of the title complex in a projection along [100]. The dashed lines indicate intermolecular hydrogen bonds. All H atoms that are not involved in these interactions have been omitted for clarity; displacement ellipsoids are drawn at the 50% probability level.

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C1—H1⋯Cl1	0.98	2.92	3.479 (5)	117
C17—H17⋯Cl2	0.98	2.65	3.323 (5)	126
N1—H1*A*⋯Cl1^{i}	0.89	2.71	3.586 (4)	168
N2—H2*A*⋯Cl2^{ii}	0.89	2.66	3.524 (4)	165
N2—H2*B*⋯Cl2^{iii}	0.89	2.63	3.355 (4)	139

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

van der Waals interactions (Steiner, 1996; Desiraju, 1996). The Pd⋯Pd separations between neighboring Pd^{II} complexes vary from 5.5027 (5) to 6.5385 (5) Å, indicating that there is no strong interaction among these metal atoms.

A search of the Cambridge Structural Database (CSD, version 5.42, current as of November 2023; Groom *et al.*, 2016) yielded thirteen related entries to the title bis(amine)–Pd^{II} complex: UMIBOH (Sui-Seng & Zargarian, 2003), UMIBOH01 (Karami *et al.*, 2018), WOCLEF (Decken *et al.*, 2000), DUKMAA (Ha, 2020), BUYCIJ (Al-Jibori *et al.*, 2015), TUWKEB (Grishin *et al.*, 2003), YEFNUT (Vazquez *et al.*, 2006), YEFNUT01 (Sabater *et al.*, 2013), GAZZAI (Kuz'mina *et al.*, 1987), GAZZEM (Kuz'mina *et al.*, 1987), PEWZEY (Karami *et al.*, 2013), POHKON (Martin *et al.*, 2008), and CUGGIU (Jones *et al.*, 1984). In the crystal structure of PEWZEY ($P2_1/c$), molecules are linked by intermolecular N—H⋯Cl hydrogen bonds into zigzag chains running parallel to the *b* axis. The asymmetric unit of GAZZEM ($P2_1$) comprises one molecule. In YEFNUT (*C*2), the amine ligands are *trans*-coordinated to a $PdCl_2$ core, and arranged in a *gauche* conformation. The asymmetric unit of TUWKEB (*C*2/*c*) comprises one molecule. In DUKMAA ($I4_1cd$), the complexes and solvent DMSO molecules are linked by N—H⋯O, N—H⋯Cl, C—H⋯Cl and C—H⋯O hydrogen bonds. The crystal structure of UMIBOH crystallizes in space group $P4_2/n$ with four independent molecules within the unit cell. The asymmetric unit of GAZZAI ($P4_32_12$) comprises one molecule. In POHKON (*P*21/*n*), the Pd^{II} atom has a distorted square-planar environment with the ligands occupying a *trans*-configuration with two molecules of dimethyl sulfoxide (DMSO) in the crystal. In the crystal structure of BUYCIJ, a hydrogen bonding interaction between the water molecule and the metal-bound chlorido ligand is present. CUGGIU comprises a Pd^{II} atom coordinated by the nitrogen atoms of four benzylamine ligands with hydrogen bonding of the N–H_2 groups with the Cl^- ion. The WOCLEF ($P2_1/n$) compound crystallizes with two molecules of DMSO and shows N—H⋯O and C—H⋯Cl hydrogen bonds between the complex and the DMSO molecules.

Synthesis and crystallization

A solution of bis(benzonitrile)palladium(II) chloride (0.66 g, 0.17 mmol) in CH_2Cl_2 (5 ml) was added to a solution of (*S*)-(+)-[1-(4-methylphenyl)-*N*-(4-biphenyl)methyliden]ethylamine (0.100 g, 0.34 mmol) in CH_2Cl_2 (10 ml). The solution was stirred for 24 h to give an orange precipitate. The solid was filtered off, dissolved in DMF, and the solution was slowly evaporated. After a few days, orange crystals were collected. Yield 23%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[PdCl_2(C_9H_{13}N)_2]$
M_r	447.71
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, b, c (Å)	6.5385 (2), 16.7263 (8), 19.0096 (11)
V (Å^3)	2078.99 (17)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.15
Crystal size (mm)	0.58 × 0.38 × 0.14
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.722, 0.915
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	45575, 7907, 5561
R_{int}	0.061
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.769
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.095, 1.05
No. of reflections	7907
No. of parameters	212
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.62, −0.64
Absolute structure	Flack x determined using 1800 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.032 (18)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXD* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

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trans-Dichloridobis[(*S*)-(−)-1-(4-methylphenyl)ethylamine-*κN*]palladium(II)

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Crystal data

$[PdCl_2(C_9H_{13}N)_2]$
M_r = 447.71
Orthorhombic, $P2_12_12_1$
a = 6.5385 (2) Å
b = 16.7263 (8) Å
c = 19.0096 (11) Å
V = 2078.99 (17) Å^3
Z = 4
F(000) = 912
D_x = 1.430 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7901 reflections
θ = 3.3–27.1°
μ = 1.15 mm^{-1}
T = 293 K
Block, yellow
0.58 × 0.38 × 0.14 mm

Data collection

Xcalibur, Atlas, Gemini diffractometer
Detector resolution: 10.5564 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.722, T_{max} = 0.915
45575 measured reflections
7907 independent reflections
5561 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 33.1°, θ_{min} = 3.3°
h = −10→10
k = −25→25
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.095
S = 1.05
7907 reflections
212 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2 + 0.5029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
Absolute structure: Flack x determined using 1800 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.032 (18)

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. The hydrogen atoms attached to carbon and nitrogen atoms were positioned with idealized geometry and constrained to ride on their parent atoms, and were refined isotropically using a riding model.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.43881 (5)	0.37662 (2)	0.46621 (2)	0.04528 (10)
Cl1	0.72228 (19)	0.43738 (10)	0.51427 (9)	0.0786 (5)
Cl2	0.14917 (17)	0.31631 (8)	0.42362 (8)	0.0618 (4)
C1	0.2846 (8)	0.5452 (3)	0.4715 (3)	0.0574 (12)
H1	0.427445	0.550708	0.456647	0.069*
C2	0.2394 (8)	0.6133 (3)	0.5206 (3)	0.0529 (11)
C3	0.3892 (9)	0.6670 (3)	0.5384 (4)	0.0700 (15)
H3	0.519174	0.660828	0.519264	0.084*
C4	0.3531 (12)	0.7299 (4)	0.5837 (4)	0.082 (2)
H4	0.458570	0.764935	0.594914	0.099*
C5	0.1610 (12)	0.7412 (3)	0.6126 (3)	0.0743 (17)
C6	0.0115 (9)	0.6873 (4)	0.5960 (3)	0.0717 (16)
H6	−0.117513	0.692942	0.616073	0.086*
C7	0.0475 (9)	0.6243 (3)	0.5499 (3)	0.0658 (13)
H7	−0.058080	0.589240	0.538736	0.079*
C8	0.1214 (15)	0.8108 (4)	0.6624 (4)	0.109 (3)
H8A	−0.020601	0.811728	0.675214	0.163*
H8B	0.156602	0.860098	0.639512	0.163*
H8C	0.203350	0.804591	0.703986	0.163*
C9	0.1548 (13)	0.5439 (4)	0.4054 (3)	0.089 (2)
H9A	0.194650	0.499443	0.376566	0.133*
H9B	0.174363	0.592758	0.379829	0.133*
H9C	0.013344	0.538613	0.418088	0.133*
C10	0.6754 (7)	0.1854 (3)	0.3317 (3)	0.0538 (12)
C11	0.5455 (8)	0.1214 (4)	0.3346 (3)	0.0696 (14)
H11	0.410391	0.129536	0.348156	0.084*
C12	0.6089 (12)	0.0453 (4)	0.3181 (4)	0.079 (2)
H12	0.515250	0.003482	0.318976	0.094*
C13	0.8098 (12)	0.0302 (4)	0.3004 (3)	0.0724 (17)
C14	0.9381 (11)	0.0941 (4)	0.2986 (4)	0.086 (2)
H14	1.074562	0.085587	0.287024	0.103*
C15	0.8753 (8)	0.1713 (4)	0.3133 (4)	0.0789 (19)
H15	0.967897	0.213352	0.310781	0.095*
C16	0.8851 (15)	−0.0534 (4)	0.2830 (4)	0.111 (3)
H16A	0.825566	−0.090992	0.315120	0.166*
H16B	1.031357	−0.055076	0.286979	0.166*
H16C	0.845891	−0.066826	0.235748	0.166*
C17	0.5914 (7)	0.2677 (3)	0.3488 (3)	0.0563 (12)
H17	0.444373	0.266492	0.338874	0.068*
C18	0.6817 (12)	0.3357 (4)	0.3063 (4)	0.0852 (19)
H18A	0.624801	0.385508	0.322108	0.128*
H18B	0.649956	0.328210	0.257422	0.128*
H18C	0.827385	0.336610	0.312394	0.128*
N1	0.2654 (6)	0.4663 (2)	0.5077 (2)	0.0496 (9)
H1A	0.134790	0.451351	0.506492	0.060*

H1B	0.299856	0.472545	0.552656	0.060*
N2	0.6156 (6)	0.2865 (2)	0.4253 (2)	0.0532 (10)
H2A	0.746127	0.298909	0.432873	0.064*
H2B	0.589351	0.242141	0.449531	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.03448 (13)	0.05194 (17)	0.04942 (17)	0.00021 (15)	−0.00095 (15)	−0.00264 (18)
Cl1	0.0396 (6)	0.1033 (11)	0.0927 (12)	−0.0090 (7)	−0.0076 (6)	−0.0358 (9)
Cl2	0.0343 (5)	0.0663 (8)	0.0849 (10)	−0.0047 (5)	−0.0015 (6)	−0.0168 (7)
C1	0.065 (3)	0.053 (3)	0.054 (3)	0.001 (2)	0.008 (3)	0.001 (3)
C2	0.062 (3)	0.046 (3)	0.051 (3)	−0.001 (2)	0.003 (2)	0.001 (2)
C3	0.075 (4)	0.061 (3)	0.074 (4)	−0.011 (3)	0.010 (3)	0.003 (3)
C4	0.107 (5)	0.061 (4)	0.080 (5)	−0.023 (4)	−0.002 (4)	−0.005 (3)
C5	0.110 (5)	0.053 (3)	0.060 (4)	0.004 (3)	−0.004 (4)	−0.003 (3)
C6	0.074 (4)	0.076 (4)	0.064 (4)	0.014 (3)	0.004 (3)	−0.005 (3)
C7	0.070 (3)	0.060 (3)	0.067 (3)	0.001 (3)	−0.009 (3)	−0.007 (3)
C8	0.169 (9)	0.079 (4)	0.079 (5)	0.006 (5)	0.005 (5)	−0.027 (4)
C9	0.139 (6)	0.073 (4)	0.054 (4)	0.022 (4)	−0.004 (4)	−0.007 (3)
C10	0.042 (2)	0.073 (3)	0.046 (3)	0.005 (2)	−0.002 (2)	−0.006 (3)
C11	0.055 (3)	0.084 (4)	0.070 (3)	0.004 (4)	0.008 (3)	0.017 (3)
C12	0.088 (5)	0.067 (4)	0.081 (5)	−0.002 (3)	0.004 (4)	0.013 (3)
C13	0.096 (5)	0.075 (4)	0.046 (3)	0.013 (4)	0.003 (3)	−0.002 (3)
C14	0.055 (3)	0.108 (5)	0.095 (5)	0.015 (4)	0.011 (4)	−0.035 (4)
C15	0.048 (3)	0.091 (4)	0.098 (5)	0.000 (3)	0.011 (3)	−0.036 (4)
C16	0.168 (9)	0.085 (5)	0.079 (5)	0.036 (6)	0.016 (5)	−0.001 (4)
C17	0.042 (3)	0.075 (3)	0.051 (3)	0.007 (2)	−0.005 (2)	−0.006 (3)
C18	0.101 (5)	0.080 (4)	0.075 (5)	0.009 (4)	0.005 (4)	0.008 (4)
N1	0.049 (2)	0.051 (2)	0.049 (2)	0.0013 (17)	0.0052 (18)	−0.0033 (18)
N2	0.0399 (19)	0.065 (2)	0.055 (3)	0.0106 (18)	0.0000 (17)	−0.005 (2)

Geometric parameters (Å, º)

Pd1—Cl1	2.3028 (13)	C10—C11	1.368 (7)
Pd1—Cl2	2.2933 (12)	C10—C15	1.373 (7)
Pd1—N1	2.039 (4)	C10—C17	1.517 (7)
Pd1—N2	2.053 (4)	C11—H11	0.9300
C1—H1	0.9800	C11—C12	1.374 (8)
C1—C2	1.502 (7)	C12—H12	0.9300
C1—C9	1.516 (9)	C12—C13	1.379 (10)
C1—N1	1.494 (6)	C13—C14	1.360 (9)
C2—C3	1.371 (7)	C13—C16	1.518 (9)
C2—C7	1.385 (7)	C14—H14	0.9300
C3—H3	0.9300	C14—C15	1.382 (8)
C3—C4	1.381 (8)	C15—H15	0.9300
C4—H4	0.9300	C16—H16A	0.9600
C4—C5	1.383 (10)	C16—H16B	0.9600

C5—C6	1.366 (9)	C16—H16C	0.9600
C5—C8	1.524 (8)	C17—H17	0.9800
C6—H6	0.9300	C17—C18	1.515 (8)
C6—C7	1.391 (8)	C17—N2	1.496 (7)
C7—H7	0.9300	C18—H18A	0.9600
C8—H8A	0.9600	C18—H18B	0.9600
C8—H8B	0.9600	C18—H18C	0.9600
C8—H8C	0.9600	N1—H1A	0.8900
C9—H9A	0.9600	N1—H1B	0.8900
C9—H9B	0.9600	N2—H2A	0.8900
C9—H9C	0.9600	N2—H2B	0.8900
Cl2—Pd1—Cl1	177.22 (6)	C10—C11—H11	119.1
N1—Pd1—Cl1	88.25 (12)	C10—C11—C12	121.9 (6)
N1—Pd1—Cl2	90.05 (12)	C12—C11—H11	119.1
N1—Pd1—N2	179.39 (18)	C11—C12—H12	119.6
N2—Pd1—Cl1	91.21 (12)	C11—C12—C13	120.9 (7)
N2—Pd1—Cl2	90.48 (12)	C13—C12—H12	119.6
C2—C1—H1	107.2	C12—C13—C16	122.1 (7)
C2—C1—C9	114.6 (4)	C14—C13—C12	116.7 (6)
C9—C1—H1	107.2	C14—C13—C16	121.2 (7)
N1—C1—H1	107.2	C13—C14—H14	118.5
N1—C1—C2	111.5 (4)	C13—C14—C15	123.1 (6)
N1—C1—C9	108.8 (5)	C15—C14—H14	118.5
C3—C2—C1	120.6 (5)	C10—C15—C14	119.7 (6)
C3—C2—C7	117.5 (5)	C10—C15—H15	120.2
C7—C2—C1	122.0 (5)	C14—C15—H15	120.2
C2—C3—H3	119.0	C13—C16—H16A	109.5
C2—C3—C4	122.1 (6)	C13—C16—H16B	109.5
C4—C3—H3	119.0	C13—C16—H16C	109.5
C3—C4—H4	119.8	H16A—C16—H16B	109.5
C3—C4—C5	120.5 (6)	H16A—C16—H16C	109.5
C5—C4—H4	119.8	H16B—C16—H16C	109.5
C4—C5—C8	120.3 (7)	C10—C17—H17	107.2
C6—C5—C4	117.9 (6)	C18—C17—C10	115.2 (5)
C6—C5—C8	121.7 (7)	C18—C17—H17	107.2
C5—C6—H6	119.2	N2—C17—C10	111.1 (4)
C5—C6—C7	121.6 (6)	N2—C17—H17	107.2
C7—C6—H6	119.2	N2—C17—C18	108.6 (5)
C2—C7—C6	120.5 (5)	C17—C18—H18A	109.5
C2—C7—H7	119.8	C17—C18—H18B	109.5
C6—C7—H7	119.8	C17—C18—H18C	109.5
C5—C8—H8A	109.5	H18A—C18—H18B	109.5
C5—C8—H8B	109.5	H18A—C18—H18C	109.5
C5—C8—H8C	109.5	H18B—C18—H18C	109.5
H8A—C8—H8B	109.5	Pd1—N1—H1A	108.5
H8A—C8—H8C	109.5	Pd1—N1—H1B	108.5
H8B—C8—H8C	109.5	C1—N1—Pd1	115.2 (3)

C1—C9—H9A	109.5	C1—N1—H1A	108.5
C1—C9—H9B	109.5	C1—N1—H1B	108.5
C1—C9—H9C	109.5	H1A—N1—H1B	107.5
H9A—C9—H9B	109.5	Pd1—N2—H2A	107.9
H9A—C9—H9C	109.5	Pd1—N2—H2B	107.9
H9B—C9—H9C	109.5	C17—N2—Pd1	117.6 (3)
C11—C10—C15	117.8 (6)	C17—N2—H2A	107.9
C11—C10—C17	118.5 (5)	C17—N2—H2B	107.9
C15—C10—C17	123.7 (5)	H2A—N2—H2B	107.2

C1—C2—C3—C4	−179.6 (6)	C11—C10—C15—C14	0.0 (10)
C1—C2—C7—C6	179.1 (5)	C11—C10—C17—C18	−144.6 (6)
C2—C1—N1—Pd1	−153.2 (3)	C11—C10—C17—N2	91.3 (6)
C2—C3—C4—C5	−0.5 (10)	C11—C12—C13—C14	−1.4 (11)
C3—C2—C7—C6	−0.6 (8)	C11—C12—C13—C16	179.1 (6)
C3—C4—C5—C6	1.4 (11)	C12—C13—C14—C15	−0.3 (11)
C3—C4—C5—C8	−179.8 (6)	C13—C14—C15—C10	1.0 (12)
C4—C5—C6—C7	−1.9 (10)	C15—C10—C11—C12	−1.7 (9)
C5—C6—C7—C2	1.5 (9)	C15—C10—C17—C18	35.4 (8)
C7—C2—C3—C4	0.1 (9)	C15—C10—C17—N2	−88.7 (7)
C8—C5—C6—C7	179.3 (6)	C16—C13—C14—C15	179.2 (7)
C9—C1—C2—C3	−120.9 (6)	C17—C10—C11—C12	178.3 (6)
C9—C1—C2—C7	59.5 (7)	C17—C10—C15—C14	180.0 (6)
C9—C1—N1—Pd1	79.5 (5)	C18—C17—N2—Pd1	70.7 (5)
C10—C11—C12—C13	2.4 (10)	N1—C1—C2—C3	115.0 (5)
C10—C17—N2—Pd1	−161.6 (3)	N1—C1—C2—C7	−64.6 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Cl1	0.98	2.92	3.479 (5)	117
C17—H17···Cl2	0.98	2.65	3.323 (5)	126
N1—H1*A*···Cl1^{i}	0.89	2.71	3.586 (4)	168
N2—H2*A*···Cl2^{ii}	0.89	2.66	3.524 (4)	165
N2—H2*B*···Cl2^{iii}	0.89	2.63	3.355 (4)	139

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