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# Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole- $\kappa^2$ N<sup>2</sup>,N<sup>3</sup>]-palladium(II)

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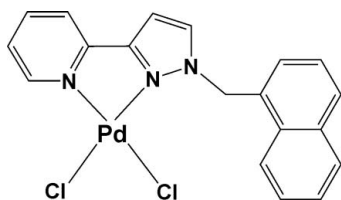
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.024;  $wR$  factor = 0.054; data-to-parameter ratio = 16.4.

In the title compound,  $[\text{PdCl}_2(\text{C}_{19}\text{H}_{15}\text{N}_3)]$ , the Pd<sup>II</sup> centre is four-coordinated by two N-atom donors from one 1-[3-(2-pyridyl)pyrazol-1-ylmethyl]naphthalene (*L*) ligand and by two Cl atoms in a distorted square-planar coordination geometry. In the crystal structure, adjacent Pd<sup>II</sup> mononuclear units form intermolecular C—H... $\pi$  interactions involving the benzene and pyridine rings of different *L* ligands and  $\pi$ – $\pi$  stacking interactions between the pyrazolyl-pyridine and naphthalene rings of neighbouring *L* ligands, with a centroid–centroid separation of 3.522 (1) Å.

## Related literature

For related literature, see: Bell *et al.* (2003); Janiak (2000); Liu, Li *et al.* (2007); Liu, Zhang *et al.* (2007); Paul *et al.* (2004); Singh *et al.* (2003); Sony & Ponnuswamy (2006); Steel (2005); Ward *et al.* (2001); Zhang *et al.* (2005); Zou *et al.* (2004).



## Experimental

## Crystal data

 $[\text{PdCl}_2(\text{C}_{19}\text{H}_{15}\text{N}_3)]$ 
 $M_r = 462.64$ 

 Orthorhombic,  $P2_12_12_1$ 
 $a = 9.330$  (6) Å

 $b = 12.139$  (8) Å

 $c = 15.918$  (11) Å

 $V = 1803$  (2) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 1.33$  mm<sup>-1</sup>
 $T = 293$  (2) K

 $0.20 \times 0.16 \times 0.12$  mm

## Data collection

Bruker SMART CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 1998)

 $T_{\min} = 0.772$ ,  $T_{\max} = 0.848$ 

10453 measured reflections

3702 independent reflections

 3340 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.028$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.024$ 
 $wR(F^2) = 0.054$ 
 $S = 1.03$ 

3702 reflections

226 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.37$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

1580 Friedel pairs

Flack parameter: 0.00 (3)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C17—H17A...Cg1 <sup>i</sup>	0.93	2.89	3.602	134
C18—H18A...Cg2 <sup>ii</sup>	0.93	3.05	3.803	139

Symmetry codes: (i)  $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, -z$ . Cg1 is the centroid of atoms C1–C5/C10 and Cg2 is the centroid of atoms Pd1/N2/C14/C15/N3.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: B12262).

## References

- Bell, Z. R., Harding, L. P. & Ward, M. D. (2003). *Chem. Commun.* pp. 2432–2433.
- Bruker (1998). SMART (Version 5.051), SAINT (Version 5.01), SADABS (Version 2.03) and SHELXTL (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
- Liu, C.-S., Li, J.-R., Zou, R.-Q., Zhou, J.-N., Shi, X.-S., Wang, J.-J. & Bu, X.-H. (2007). *J. Mol. Struct.* **843**, 66–77.
- Liu, C.-S., Zhang, H., Chen, R., Shi, X.-S., Bu, X.-H. & Yang, M. (2007). *Chem. Pharm. Bull.* **55**, 996–1001.
- Paul, R. L., Argent, S. P., Jeffery, J. C., Harding, L. P., Lynamd, J. M. & Ward, M. D. (2004). *J. Chem. Soc. Dalton Trans.* pp. 3453–3458.
- Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.
- Singh, S., Mishra, V., Mukherjee, J., Seethalekshmi, N. & Mukherjee, R. (2003). *J. Chem. Soc. Dalton Trans.* pp. 3392–3397.
- Sony, S. M. M. & Ponnuswamy, M. N. (2006). *Cryst. Growth Des.* **6**, 736–742.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Steel, P. J. (2005). *Acc. Chem. Res.* **38**, 243–250.
- Ward, M. D., McCleverty, J. A. & Jeffery, J. C. (2001). *Coord. Chem. Rev.* **222**, 251–272.
- Zhang, H., Liu, C.-S., Bu, X.-H. & Yang, M. (2005). *J. Inorg. Biochem.* **99**, 1119–1125.
- Zou, R.-Q., Bu, X.-H. & Zhang, R.-H. (2004). *Inorg. Chem.* **43**, 5382–5386.

## supporting information

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## Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1*H*-pyrazole- $\kappa^2N^2,N^3$ ]palladium(II)

Chun-Sen Liu, Guang-Hui Sun and Liang-Qi Guo

### S1. Comment

In recent years, attention has been focused on the synthetic approach and the structural control of metal-organic coordination architectures with ligands based on pyrazolyl-pyridine chelating units (Steel, 2005; Ward *et al.*, 2001). In this field, Ward and co-workers have reported novel functional complexes through the use of 3-(2-pyridyl)pyrazole and/or 3-(2-pyridyl)pyrazole-based ligands (Bell *et al.*, 2003; Paul *et al.*, 2004; Singh *et al.*, 2003; Ward *et al.*, 2001; Zou *et al.*, 2004). Recently, we have reported the preparation of a non-planar ligand, 1-[3-(2-pyridyl)pyrazol-1-ylmethyl]-naphthalene (denoted *L*) (Liu & Li *et al.*, 2007; Liu & Zhang *et al.*, 2007; Zhang *et al.*, 2005). We report here the crystal structure of a palladium complex of this ligand, [(*L*)PdCl<sub>2</sub>].

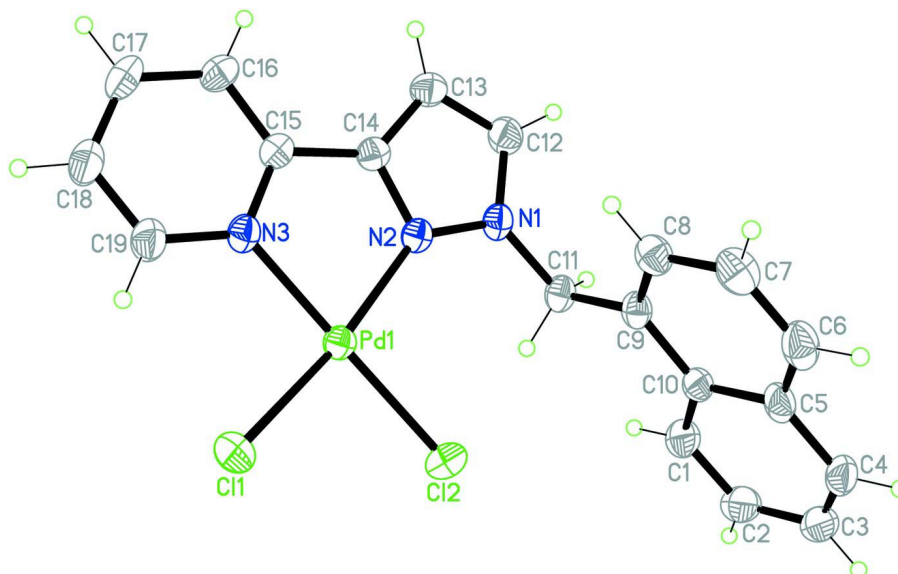
In the title compound, the Pd<sup>II</sup> centre is four-coordinated by two N-atom donors from one *L* ligand and two Cl atoms. The coordination geometry around the Pd<sup>II</sup> center can be described as a slightly distorted square-plane (Fig. 1). In the crystal structure, the Pd<sup>II</sup> mononuclear units form intermolecular  $\pi\cdots\pi$  stacking interactions between pyrazolyl-pyridine and naphthalene rings of neighbouring *L* ligands with a centroid-centroid separation of 3.522 (1) Å (Janiak, 2000) and C—H $\cdots\pi$  interactions involving C1/C2/C3/C4/C5/C10 (centroid *Cg*1) benzene rings of the *L* ligands as well as five-membered chelate rings Pd1/N2/C14/C15/N3 (centroid *Cg*2) (Sony and Ponnuswamy, 2006) (Fig. 2).

### S2. Experimental

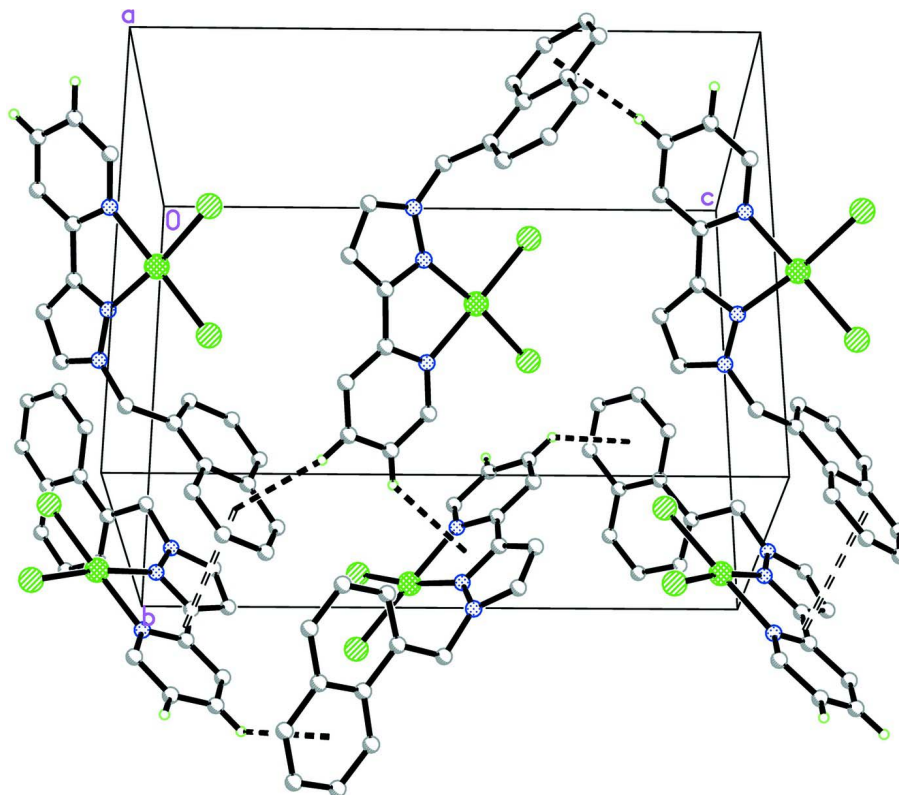
The ligand 1-[3-(2-pyridyl)pyrazol-1-ylmethyl]naphthalene (*L*) was synthesized according to the method reported in the literature (Liu & Li *et al.*, 2007; Liu & Zhang *et al.*, 2007; Zhang *et al.*, 2005). A solution of PdCl<sub>2</sub> (0.1 mmol) in methanol (15 ml) and acetonitrile (5 ml) was added to *L* (0.1 mmol). A yellow solid formed was filtered off and the resulting solution was kept at room temperature. Yellow single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days. Yield: *ca* 30%. Elemental analysis calculated: C 49.32, H 3.27, N 9.08%; found: C 49.47, H 3.16, N 9.20%.

### S3. Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5 U_{\text{eq}}(\text{C})$ .

**Figure 1**

Molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

**Figure 2**

Part of the crystal packing showing a two-dimensional network structure in the title compound formed by the co-effects of intermolecular C—H... $\pi$  (dashed solid lines) and  $\pi$ ... $\pi$  stacking (dashed open lines) interactions. For the sake of clarity, only H atoms involved in the interactions are shown.

Dichlorido[1-(1-naphthylmethyl)-3-(2-pyridyl)-1H-pyrazole- $\kappa^2N^2,N^3$ ]palladium(II)

## Crystal data

[PdCl<sub>2</sub>(C<sub>19</sub>H<sub>15</sub>N<sub>3</sub>)] $M_r = 462.64$ Orthorhombic,  $P2_12_12_1$ 

Hall symbol: P 2ac 2ab

 $a = 9.330$  (6) Å $b = 12.139$  (8) Å $c = 15.918$  (11) Å $V = 1803$  (2) Å<sup>3</sup> $Z = 4$  $F(000) = 920$  $D_x = 1.705$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 970 reflections

 $\theta = 3.4$ – $26.4^\circ$  $\mu = 1.33$  mm<sup>-1</sup> $T = 293$  K

Block, yellow

 $0.20 \times 0.16 \times 0.12$  mm

## Data collection

Bruker SMART CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 1998)

 $T_{\min} = 0.772$ ,  $T_{\max} = 0.848$ 

10453 measured reflections

3702 independent reflections

3340 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.028$  $\theta_{\max} = 26.5^\circ$ ,  $\theta_{\min} = 2.5^\circ$  $h = -10 \rightarrow 11$  $k = -14 \rightarrow 15$  $l = -19 \rightarrow 15$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.024$  $wR(F^2) = 0.054$  $S = 1.03$ 

3702 reflections

226 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

 $w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 0.3859P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.27$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.37$  e Å<sup>-3</sup>Absolute structure: Flack (1983), 1580 Friedel  
pairs

Absolute structure parameter: 0.00 (3)

## 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<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd1	0.83064 (2)	0.490954 (17)	0.051890 (13)	0.03837 (7)
C1	0.5698 (4)	0.9043 (3)	0.1086 (3)	0.0546 (9)
H1A	0.6381	0.9001	0.0662	0.065*

C2	0.5637 (4)	0.9961 (3)	0.1585 (3)	0.0654 (10)
H2A	0.6281	1.0534	0.1498	0.079*
C3	0.4620 (4)	1.0044 (4)	0.2221 (2)	0.0704 (12)
H3A	0.4589	1.0670	0.2557	0.084*
C4	0.3679 (4)	0.9219 (4)	0.2351 (2)	0.0651 (11)
H4A	0.2993	0.9290	0.2771	0.078*
C5	0.3714 (3)	0.8245 (3)	0.1859 (2)	0.0511 (9)
C6	0.2756 (4)	0.7376 (4)	0.1995 (2)	0.0639 (11)
H6A	0.2078	0.7433	0.2421	0.077*
C7	0.2800 (4)	0.6453 (3)	0.1516 (3)	0.0613 (10)
H7A	0.2168	0.5878	0.1622	0.074*
C8	0.3806 (4)	0.6365 (3)	0.0856 (2)	0.0505 (8)
H8A	0.3824	0.5730	0.0530	0.061*
C9	0.4752 (3)	0.7192 (2)	0.0689 (2)	0.0408 (7)
C10	0.4739 (3)	0.8161 (3)	0.1208 (2)	0.0430 (7)
C11	0.5803 (3)	0.7164 (2)	-0.0027 (2)	0.0444 (8)
H11A	0.5576	0.7758	-0.0412	0.053*
H11B	0.6756	0.7301	0.0193	0.053*
C12	0.5032 (4)	0.5886 (3)	-0.1173 (2)	0.0534 (8)
H12A	0.4323	0.6329	-0.1406	0.064*
C13	0.5448 (3)	0.4872 (3)	-0.1465 (2)	0.0512 (8)
H13A	0.5090	0.4492	-0.1927	0.061*
C14	0.6522 (3)	0.4540 (2)	-0.09185 (19)	0.0397 (7)
C15	0.7469 (3)	0.3595 (2)	-0.0911 (2)	0.0394 (7)
C16	0.7465 (4)	0.2785 (3)	-0.1518 (2)	0.0479 (8)
H16A	0.6799	0.2806	-0.1952	0.058*
C17	0.8446 (4)	0.1953 (3)	-0.1477 (3)	0.0612 (10)
H17A	0.8459	0.1404	-0.1885	0.073*
C18	0.9416 (5)	0.1935 (3)	-0.0826 (3)	0.0675 (13)
H18A	1.0096	0.1377	-0.0789	0.081*
C19	0.9366 (4)	0.2753 (3)	-0.0231 (3)	0.0619 (11)
H19A	1.0022	0.2740	0.0209	0.074*
N1	0.5823 (3)	0.6132 (2)	-0.04930 (19)	0.0434 (6)
N2	0.6739 (3)	0.53078 (17)	-0.03249 (14)	0.0378 (5)
N3	0.8397 (3)	0.35759 (19)	-0.02653 (16)	0.0438 (6)
Cl1	1.00048 (11)	0.42155 (9)	0.13879 (7)	0.0708 (3)
Cl2	0.81909 (11)	0.64162 (6)	0.13707 (5)	0.0521 (2)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pd1	0.03920 (11)	0.03896 (11)	0.03696 (11)	0.00037 (11)	0.00213 (10)	0.00045 (11)
C1	0.058 (2)	0.0449 (19)	0.060 (2)	0.0110 (17)	-0.0040 (18)	0.0000 (17)
C2	0.075 (2)	0.0455 (19)	0.076 (3)	0.013 (2)	-0.024 (2)	-0.010 (2)
C3	0.077 (3)	0.066 (3)	0.068 (2)	0.035 (3)	-0.030 (2)	-0.022 (2)
C4	0.062 (3)	0.083 (3)	0.051 (2)	0.038 (2)	-0.0089 (18)	-0.015 (2)
C5	0.043 (2)	0.064 (2)	0.045 (2)	0.0218 (16)	-0.0049 (15)	0.0039 (17)
C6	0.054 (2)	0.091 (3)	0.047 (2)	0.019 (2)	0.0085 (18)	0.009 (2)

C7	0.052 (2)	0.067 (3)	0.065 (3)	-0.0033 (18)	0.0031 (19)	0.016 (2)
C8	0.0479 (19)	0.0458 (18)	0.058 (2)	0.0036 (15)	-0.0020 (16)	0.0069 (16)
C9	0.0423 (17)	0.0381 (15)	0.0422 (19)	0.0102 (13)	0.0011 (15)	0.0071 (13)
C10	0.0429 (18)	0.0443 (17)	0.0417 (18)	0.0133 (14)	-0.0067 (14)	-0.0004 (14)
C11	0.0485 (19)	0.0372 (17)	0.048 (2)	0.0078 (15)	0.0034 (15)	0.0021 (16)
C12	0.056 (2)	0.060 (2)	0.045 (2)	0.0141 (18)	-0.0071 (18)	0.0007 (16)
C13	0.0554 (18)	0.057 (2)	0.0416 (17)	0.0038 (19)	-0.0077 (14)	-0.0047 (18)
C14	0.0411 (17)	0.0422 (15)	0.0357 (16)	-0.0023 (14)	0.0045 (14)	0.0002 (12)
C15	0.0440 (18)	0.0360 (16)	0.0381 (18)	-0.0043 (14)	0.0079 (14)	0.0011 (13)
C16	0.058 (2)	0.0444 (19)	0.041 (2)	-0.0048 (15)	0.0079 (16)	-0.0053 (15)
C17	0.075 (3)	0.0427 (18)	0.065 (2)	0.005 (2)	0.015 (3)	-0.0149 (16)
C18	0.074 (3)	0.055 (2)	0.073 (3)	0.022 (2)	-0.002 (2)	-0.013 (2)
C19	0.070 (3)	0.054 (2)	0.062 (3)	0.0214 (19)	-0.011 (2)	-0.0067 (17)
N1	0.0465 (15)	0.0424 (13)	0.0414 (15)	0.0105 (11)	0.0035 (13)	0.0016 (14)
N2	0.0408 (12)	0.0366 (11)	0.0361 (13)	0.0021 (11)	0.0040 (11)	0.0018 (9)
N3	0.0489 (15)	0.0385 (12)	0.0440 (15)	0.0071 (14)	0.0022 (14)	0.0013 (10)
Cl1	0.0659 (6)	0.0788 (6)	0.0677 (6)	0.0211 (5)	-0.0224 (5)	-0.0102 (5)
Cl2	0.0678 (5)	0.0452 (4)	0.0435 (4)	-0.0047 (4)	0.0009 (5)	-0.0056 (3)

*Geometric parameters (Å, °)*

Pd1—N2	2.043 (3)	C9—C11	1.504 (5)
Pd1—N3	2.046 (3)	C11—N1	1.456 (4)
Pd1—Cl1	2.2658 (14)	C11—H11A	0.970
Pd1—Cl2	2.2792 (14)	C11—H11B	0.970
C1—C2	1.370 (5)	C12—N1	1.343 (5)
C1—C10	1.408 (5)	C12—C13	1.372 (5)
C1—H1A	0.930	C12—H12A	0.930
C2—C3	1.390 (6)	C13—C14	1.387 (4)
C2—H2A	0.930	C13—H13A	0.930
C3—C4	1.347 (6)	C14—N2	1.342 (4)
C3—H3A	0.930	C14—C15	1.448 (4)
C4—C5	1.418 (5)	C15—N3	1.343 (4)
C4—H4A	0.930	C15—C16	1.379 (4)
C5—C6	1.399 (5)	C16—C17	1.365 (5)
C5—C10	1.414 (5)	C16—H16A	0.930
C6—C7	1.356 (6)	C17—C18	1.377 (6)
C6—H6A	0.930	C17—H17A	0.930
C7—C8	1.413 (5)	C18—C19	1.373 (5)
C7—H7A	0.930	C18—H18A	0.930
C8—C9	1.363 (5)	C19—N3	1.348 (4)
C8—H8A	0.930	C19—H19A	0.930
C9—C10	1.438 (4)	N1—N2	1.343 (3)
N2—Pd1—N3	79.38 (10)	C9—C11—H11A	108.7
N2—Pd1—Cl1	171.74 (7)	N1—C11—H11B	108.7
N3—Pd1—Cl1	92.83 (9)	C9—C11—H11B	108.7
N2—Pd1—Cl2	99.63 (7)	H11A—C11—H11B	107.6

N3—Pd1—C12	178.86 (7)	N1—C12—C13	108.5 (3)
C11—Pd1—C12	88.18 (5)	N1—C12—H12A	125.8
C2—C1—C10	120.8 (4)	C13—C12—H12A	125.8
C2—C1—H1A	119.6	C12—C13—C14	104.6 (3)
C10—C1—H1A	119.6	C12—C13—H13A	127.7
C1—C2—C3	120.6 (4)	C14—C13—H13A	127.7
C1—C2—H2A	119.7	N2—C14—C13	110.4 (3)
C3—C2—H2A	119.7	N2—C14—C15	116.8 (3)
C4—C3—C2	120.2 (4)	C13—C14—C15	132.6 (3)
C4—C3—H3A	119.9	N3—C15—C16	121.7 (3)
C2—C3—H3A	119.9	N3—C15—C14	114.4 (3)
C3—C4—C5	121.3 (4)	C16—C15—C14	123.9 (3)
C3—C4—H4A	119.3	C17—C16—C15	119.5 (4)
C5—C4—H4A	119.3	C17—C16—H16A	120.2
C6—C5—C10	119.4 (3)	C15—C16—H16A	120.2
C6—C5—C4	121.9 (4)	C16—C17—C18	119.2 (3)
C10—C5—C4	118.6 (4)	C16—C17—H17A	120.4
C7—C6—C5	121.1 (4)	C18—C17—H17A	120.4
C7—C6—H6A	119.5	C19—C18—C17	119.1 (4)
C5—C6—H6A	119.5	C19—C18—H18A	120.5
C6—C7—C8	120.1 (4)	C17—C18—H18A	120.5
C6—C7—H7A	120.0	N3—C19—C18	122.0 (4)
C8—C7—H7A	120.0	N3—C19—H19A	119.0
C9—C8—C7	121.3 (3)	C18—C19—H19A	119.0
C9—C8—H8A	119.4	C12—N1—N2	110.2 (3)
C7—C8—H8A	119.4	C12—N1—C11	126.5 (3)
C8—C9—C10	119.0 (3)	N2—N1—C11	123.2 (3)
C8—C9—C11	123.6 (3)	C14—N2—N1	106.3 (2)
C10—C9—C11	117.3 (3)	C14—N2—Pd1	113.99 (19)
C1—C10—C5	118.5 (3)	N1—N2—Pd1	139.7 (2)
C1—C10—C9	122.5 (3)	C15—N3—C19	118.4 (3)
C5—C10—C9	119.1 (3)	C15—N3—Pd1	115.2 (2)
N1—C11—C9	114.4 (3)	C19—N3—Pd1	126.1 (2)
N1—C11—H11A	108.7		
C10—C1—C2—C3	-0.3 (5)	C14—C15—C16—C17	176.9 (3)
C1—C2—C3—C4	-0.2 (6)	C15—C16—C17—C18	0.4 (6)
C2—C3—C4—C5	1.1 (6)	C16—C17—C18—C19	0.3 (6)
C3—C4—C5—C6	179.1 (3)	C17—C18—C19—N3	-0.1 (7)
C3—C4—C5—C10	-1.6 (5)	C13—C12—N1—N2	-0.4 (4)
C10—C5—C6—C7	0.4 (5)	C13—C12—N1—C11	175.1 (3)
C4—C5—C6—C7	179.6 (4)	C9—C11—N1—C12	90.9 (4)
C5—C6—C7—C8	-1.2 (6)	C9—C11—N1—N2	-94.1 (3)
C6—C7—C8—C9	0.4 (6)	C13—C14—N2—N1	-0.6 (3)
C7—C8—C9—C10	1.3 (5)	C15—C14—N2—N1	175.4 (2)
C7—C8—C9—C11	-177.3 (3)	C13—C14—N2—Pd1	-179.9 (2)
C2—C1—C10—C5	-0.2 (5)	C15—C14—N2—Pd1	-3.9 (3)
C2—C1—C10—C9	178.9 (3)	C12—N1—N2—C14	0.6 (3)



C6—C5—C10—C1	-179.6 (3)	C11—N1—N2—C14	-175.1 (3)
C4—C5—C10—C1	1.1 (5)	C12—N1—N2—Pd1	179.6 (2)
C6—C5—C10—C9	1.3 (5)	C11—N1—N2—Pd1	4.0 (5)
C4—C5—C10—C9	-178.0 (3)	N3—Pd1—N2—C14	2.0 (2)
C8—C9—C10—C1	178.8 (3)	C12—Pd1—N2—C14	-178.62 (19)
C11—C9—C10—C1	-2.5 (5)	N3—Pd1—N2—N1	-177.0 (3)
C8—C9—C10—C5	-2.1 (5)	C12—Pd1—N2—N1	2.4 (3)
C11—C9—C10—C5	176.6 (3)	C16—C15—N3—C19	1.7 (5)
C8—C9—C11—N1	-5.1 (5)	C14—C15—N3—C19	-176.8 (3)
C10—C9—C11—N1	176.2 (3)	C16—C15—N3—Pd1	176.1 (2)
N1—C12—C13—C14	0.0 (4)	C14—C15—N3—Pd1	-2.4 (3)
C12—C13—C14—N2	0.3 (4)	C18—C19—N3—C15	-0.9 (6)
C12—C13—C14—C15	-174.8 (3)	C18—C19—N3—Pd1	-174.7 (3)
N2—C14—C15—N3	4.2 (4)	N2—Pd1—N3—C15	0.3 (2)
C13—C14—C15—N3	179.2 (3)	C11—Pd1—N3—C15	177.6 (2)
N2—C14—C15—C16	-174.3 (3)	N2—Pd1—N3—C19	174.2 (3)
C13—C14—C15—C16	0.7 (6)	C11—Pd1—N3—C19	-8.5 (3)
N3—C15—C16—C17	-1.5 (5)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C17—H17 <i>A</i> ...C <i>g</i> 1 <sup>i</sup>	0.93	2.89	3.602	134
C18—H18 <i>A</i> ...C <i>g</i> 2 <sup>ii</sup>	0.93	3.05	3.803	139

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