Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# {μ-1,3-Bis[(3,5-dimethylpyrazol-1-yl)-methyl]benzene-κ²N²:N²'}di-μ-chlorido-bis[chloridopalladium(II)] toluene solvate

**Bernard Omondi,* Asheena Budhai and James Darkwa**

Department of Chemistry, University of Johannesburg, PO Box 524, Auckland Park, 2006 Johannesburg, South Africa
Correspondence e-mail: bernardowaga@gmail.com

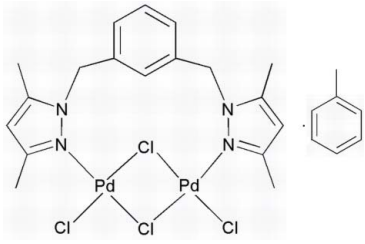
Received 17 March 2009; accepted 23 March 2009

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.042; $wR$ factor = 0.098; data-to-parameter ratio = 22.3.

In the title complex, $[Pd_2Cl_4(C_{18}H_{22}N_4)]\cdot C_7H_8$, each of the two four-coordinated $Pd^{II}$ atoms is in a slightly distorted square-planar geometry, defined by one N atom from the ligand, two bridging Cl atoms and one terminal Cl atom. Intermolecular C—H$\cdots\pi$ interactions between the pyrazole ring H atom and the toluene ring stabilize the crystal structure.

## Related literature

For general background to poly(pyrazol-1-yl-methyl)benzene ligands and their palladium complexes, see: Hartshorn & Steel (1995, 1997, 1998); Motsoane *et al.* (2007); Yen *et al.* (2006). For related structures, see: Guzei *et al.* (2003).




## Experimental

### Crystal data

$[Pd_2Cl_4(C_{18}H_{22}N_4)]\cdot C_7H_8$
$M_r$ = 741.13
Monoclinic, $P2_1/n$
$a$ = 10.4572 (10) Å
$b$ = 25.376 (2) Å
$c$ = 12.0782 (12) Å
$\beta$ = 112.395 (4)°
$V$ = 2963.4 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.60 mm$^{-1}$
$T$ = 298 K
0.50 × 0.12 × 0.06 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.503, $T_{max}$ = 0.910
22587 measured reflections
7158 independent reflections
4777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
$S$ = 1.02
7158 reflections
321 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| N2—Pd1 | 2.005 (3) | Cl3—Pd2 | 2.3421 (11) |
| N4—Pd2 | 2.002 (3) | Cl3—Pd1 | 2.3502 (10) |
| Cl1—Pd1 | 2.2647 (11) | Cl4—Pd2 | 2.3092 (11) |
| Cl2—Pd2 | 2.2774 (12) | Cl4—Pd1 | 2.3135 (12) |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C16—H16$\cdots Cg1^{i}$ | 0.93 | 2.93 | 3.802 (6) | 157 |

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$. $Cg1$ is the centroid of the C20–C25 ring.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the University of Johannesburg and the National Research Foundation (South Africa) for financial support for this project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2189).

## References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Guzei, I. A., Li, K., Bikzhanova, G. A., Darkwa, J. & Mapolie, S. F. (2003). *Dalton Trans.* pp. 715–717.
Hartshorn, C. M. & Steel, P. J. (1995). *J. Aust. Chem.* **48**, 1587–1591.
Hartshorn, C. M. & Steel, P. J. (1997). *Chem. Commun.* pp. 541–542.
Hartshorn, C. M. & Steel, P. J. (1998). *Organometallics*, **17**, 3487–3496.
Motsoane, N. M., Guzei, I. A. & Darkwa, J. (2007). *Z. Naturforsch. Teil B*, **62**, 323–330.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yen, S. K., Koh, L. L., Hahn, F. E., Huynh, H. V. & Hor, T. S. A. (2006). *Organometallics*, **25**, 5112–5118.

# supporting information

*Acta Cryst.* (2009). E**65**, m446 [doi:10.1107/S1600536809010629]

# {$\mu$-1,3-Bis[(3,5-dimethylpyrazol-1-yl)methyl]benzene-$\kappa^2N^2$:$N^{2'}$}di-$\mu$-chlorido-bis-[chloridopalladium(II)] toluene solvate

**Bernard Omondi, Asheena Budhai and James Darkwa**

## S1. Comment

The title compound is of interest as part of a study of poly(pyrazol-1-yl-methyl)benzene palladium complexes as catalyst precursors for olefin oligomerization and polymerization. In a recent report (Motsoane *et al.*, 2007), coordination of Pd atom was shown to vary depending on the position of the pyrazol-1-yl-methyl group on the benzene linker. Poly(pyrazol-1-yl-methyl)benzene ligands can coordinate to Pd atoms through two independent pyrazolyl units (Motsoane *et al.*, 2007) or as a chelate ligand to a dinuclear unit with two bridging halides between the Pd atoms in a $Pd_2X_4$ ($X$ = Cl) fashion (Yen *et al.*, 2006). This potential of poly(pyrazol-1-yl-methyl)benzene ligands exhibiting a variety of coordination modes was first reported in 1995 (Hartshorn & Steel, 1995). For the palladium complexes, two bonding modes have been reported. The first is a cage structure with six $PdCl_2$ units and four 1,3,5-tris(pyrazol-1-yl-methyl)-2,4,6-triethylbenzene ligands, with coordination through the pyrazole N atoms (Hartshorn & Steel, 1997), and the second involves C—H activation, where coordination is through a pyrazole N atom as well as through the activated C atom (Hartshorn & Steel, 1998).

The title compound (Fig. 1) crystallizes from a mixture of chloroform and toluene and contains a dinuclear Pd complex molecule and a solvent toluene molecule in the asymmetric unit. The two $Pd^{II}$ atoms are bridged by two Cl atoms. There are examples of similar structures in the literature, where the metal centers are bridged by halogen atoms (Cl or Br) (Guzei *et al.*, 2003; Motsoane *et al.*, 2007). Each of the Pd atoms has a distorted square-planar geometry (Table 1). The two square planes defined by the atoms around the Pd centers, N2, Cl1, Cl3, Cl4 for Pd1 and N4, Cl2, Cl3,Cl4 for Pd2, have a dihedral angle of 39.59 (1)° and atomic deviations from the planes of 0.018 and 0.011 Å, respectively. This dihedral angle results in a close contact between the two Pd centers [3.2116 (5) Å] and is probably due to steric bulk of the whole complex. The terminal as well as bridging Pd—Cl distances average 2.310 Å, which is close to the same distances of similar structues from the CSD (Guzei *et al.*, 2003; Motsoane *et al.*, 2007). The Pd—N bond distances [2.005 (3) and 2.002 (3) Å] are shorter than the corresponding distances from the CSD (2.1 (1) Å), as calculated by Guzei *et al.* (2003).

In the crystal structure, the dinuclear complex molecule is connected to the toluene molecule through a C—H$\cdots\pi$ interaction, with an H16$\cdots\pi$ distance of 2.93 Å (Fig. 2).

## S2. Experimental

To a solution of $PdCl_2(NCMe)_2$ (0.44 g, 1.70 mmol) in $CH_2Cl_2$ (25 mL) was added 1,3-bis[(3,5-dimethylpyrazole-1-yl)methyl]benzene (0.50 g, 1.70 mmol). The resultant solution was stired overnight, and after removal of solvent, a dark orange solid was obtained. Recrystallization was done in a mixture of $CHCl_3$ and toluene, giving needle-shaped crystals.

### S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 ($CH_2$) and 0.96 ($CH_3$) Å and with $U_{iso}$(H) = 1.2(or 1.5 for methyl)$U_{eq}$(C).

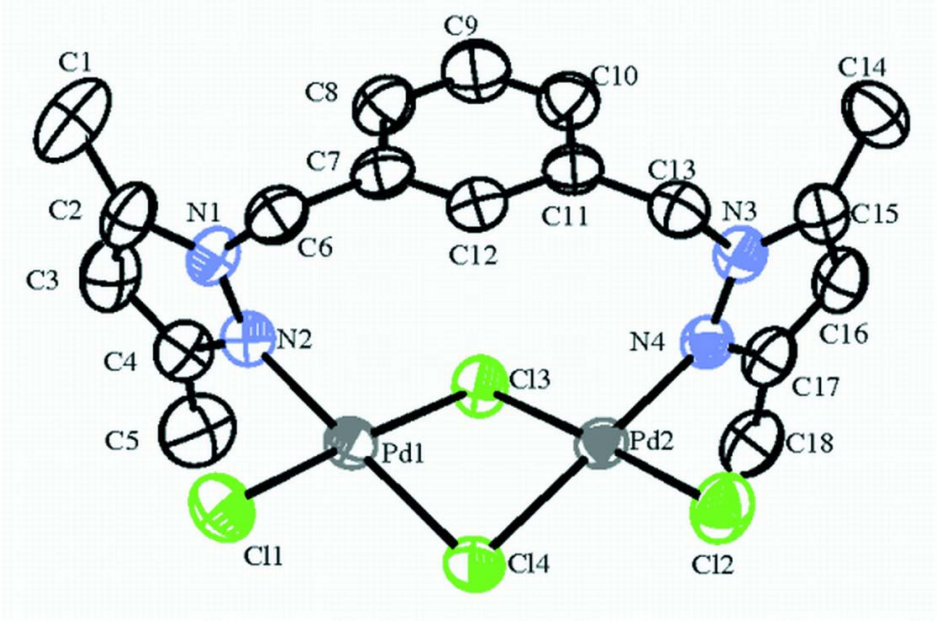



**Figure 1**

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms and toluene molecule have been omitted for clarity.

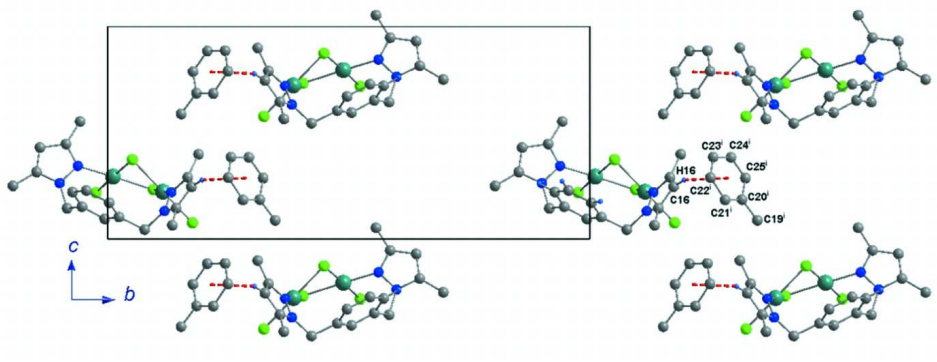



**Figure 2**

Packing diagram of the title compound, showing the intermolecular C—H···$\pi$ interactions (dashed lines) linking the Pd complex and the toluene solvent molecule. [Symmetry code: (i) 1/2+x, 3/2-y, -1/2+z.]

### {$\mu$-1,3-Bis[(3,5-dimethylpyrazol-1-yl)methyl]benzene-$\kappa^2N^2$:$N^{2'}$}di-$\mu$- chlorido-bis[chloridopalladium(II)] toluene solvate

*Crystal data*

$[Pd_2Cl_4(C_{18}H_{22}N_4)]\cdot C_7H_8$
$M_r$ = 741.13
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a$ = 10.4572 (10) Å
$b$ = 25.376 (2) Å

$c$ = 12.0782 (12) Å
$\beta$ = 112.395 (4)°
$V$ = 2963.4 (5) Å$^3$
$Z$ = 4
$F$(000) = 1472
$D_x$ = 1.661 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 22587 reflections
$\theta$ = 2.0–28.0°
$\mu$ = 1.60 mm$^{-1}$
$T$ = 298 K
Needle, brown
0.50 × 0.12 × 0.06 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.503, $T_{max}$ = 0.910

22587 measured reflections
7158 independent reflections
4777 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045
$\theta_{max}$ = 28.0°, $\theta_{min}$ = 2.0°
$h$ = −13→13
$k$ = −24→33
$l$ = −10→15

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
$S$ = 1.02
7158 reflections
321 parameters

10 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 1.0406P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1871 (7) | 0.8038 (2) | 0.2496 (6) | 0.099 (2) |
| H1A | 0.1059 | 0.8010 | 0.1775 | 0.149* |
| H1B | 0.1931 | 0.7738 | 0.2996 | 0.149* |
| H1C | 0.2676 | 0.8052 | 0.2297 | 0.149* |
| C2 | 0.1790 (5) | 0.85270 (18) | 0.3147 (5) | 0.0595 (13) |
| C3 | 0.1918 (5) | 0.8599 (2) | 0.4306 (5) | 0.0695 (14) |
| H3 | 0.2075 | 0.8337 | 0.4882 | 0.083* |
| C4 | 0.1771 (4) | 0.9140 (2) | 0.4470 (4) | 0.0571 (11) |
| C5 | 0.1804 (7) | 0.9431 (2) | 0.5530 (5) | 0.0889 (18) |
| H5A | 0.1983 | 0.9797 | 0.5444 | 0.133* |
| H5B | 0.2522 | 0.9291 | 0.6231 | 0.133* |
| H5C | 0.0928 | 0.9396 | 0.5609 | 0.133* |
| C6 | 0.1524 (4) | 0.91608 (18) | 0.1445 (4) | 0.0514 (11) |
| H6A | 0.0709 | 0.9376 | 0.1051 | 0.062* |
| H6B | 0.1445 | 0.8848 | 0.0963 | 0.062* |
| C7 | 0.2807 (4) | 0.94690 (18) | 0.1525 (4) | 0.0471 (11) |
| C8 | 0.4127 (5) | 0.9274 (2) | 0.2212 (5) | 0.0604 (13) |
| H8 | 0.4225 | 0.8955 | 0.2615 | 0.073* |
| C9 | 0.5274 (5) | 0.9558 (2) | 0.2283 (5) | 0.0695 (15) |
| H9 | 0.6151 | 0.9428 | 0.2727 | 0.083* |
| C10 | 0.5141 (4) | 1.0033 (2) | 0.1707 (5) | 0.0576 (13) |
| H10 | 0.5928 | 1.0220 | 0.1764 | 0.069* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.3838 (4) | 1.02362 (17) | 0.1036 (4) | 0.0450 (10) |
| C12 | 0.2680 (4) | 0.99412 (17) | 0.0948 (4) | 0.0433 (10) |
| H12 | 0.1803 | 1.0068 | 0.0488 | 0.052* |
| C13 | 0.3681 (4) | 1.07703 (17) | 0.0446 (4) | 0.0494 (11) |
| H13A | 0.4033 | 1.0755 | −0.0189 | 0.059* |
| H13B | 0.2709 | 1.0862 | 0.0090 | 0.059* |
| C14 | 0.6392 (5) | 1.1343 (2) | 0.0648 (5) | 0.0722 (15) |
| H14A | 0.6685 | 1.0983 | 0.0691 | 0.108* |
| H14B | 0.7187 | 1.1570 | 0.0893 | 0.108* |
| H14C | 0.5796 | 1.1426 | −0.0160 | 0.108* |
| C15 | 0.5632 (4) | 1.14228 (18) | 0.1452 (4) | 0.0493 (11) |
| C16 | 0.5951 (4) | 1.17376 (19) | 0.2460 (4) | 0.0579 (13) |
| H16 | 0.6714 | 1.1958 | 0.2780 | 0.070* |
| C17 | 0.4926 (4) | 1.16631 (17) | 0.2904 (4) | 0.0501 (11) |
| C18 | 0.4749 (5) | 1.1888 (2) | 0.3991 (5) | 0.0672 (14) |
| H18A | 0.3803 | 1.1991 | 0.3784 | 0.101* |
| H18B | 0.5339 | 1.2189 | 0.4271 | 0.101* |
| H18C | 0.4993 | 1.1626 | 0.4611 | 0.101* |
| N1 | 0.1581 (3) | 0.90068 (14) | 0.2629 (3) | 0.0473 (9) |
| N2 | 0.1594 (3) | 0.93824 (14) | 0.3438 (3) | 0.0446 (8) |
| N3 | 0.4434 (3) | 1.11796 (13) | 0.1316 (3) | 0.0453 (8) |
| N4 | 0.3997 (3) | 1.13181 (13) | 0.2198 (3) | 0.0435 (8) |
| Cl1 | −0.12855 (10) | 0.97616 (5) | 0.21818 (11) | 0.0614 (3) |
| Cl2 | 0.11537 (12) | 1.17589 (5) | 0.07665 (12) | 0.0656 (3) |
| Cl3 | 0.30569 (10) | 1.05135 (4) | 0.37297 (10) | 0.0524 (3) |
| Cl4 | 0.00312 (10) | 1.09512 (5) | 0.23267 (12) | 0.0601 (3) |
| Pd1 | 0.08672 (3) | 1.011252 (13) | 0.29434 (3) | 0.04228 (10) |
| Pd2 | 0.21405 (3) | 1.114894 (13) | 0.22275 (3) | 0.04230 (10) |
| C19 | 0.2046 (12) | 0.1522 (5) | 0.5868 (12) | 0.230 (7) |
| H19A | 0.1707 | 0.1732 | 0.5154 | 0.345* |
| H19B | 0.1281 | 0.1360 | 0.5992 | 0.345* |
| H19C | 0.2650 | 0.1253 | 0.5785 | 0.345* |
| C20 | 0.2793 (10) | 0.1850 (4) | 0.6875 (11) | 0.136 (3) |
| C21 | 0.3754 (11) | 0.2193 (4) | 0.6843 (11) | 0.147 (4) |
| H21 | 0.3940 | 0.2233 | 0.6154 | 0.177* |
| C22 | 0.4488 (12) | 0.2496 (5) | 0.7898 (14) | 0.165 (5) |
| H22 | 0.5158 | 0.2736 | 0.7892 | 0.198* |
| C23 | 0.4229 (9) | 0.2439 (4) | 0.8855 (11) | 0.149 (4) |
| H23 | 0.4704 | 0.2636 | 0.9538 | 0.179* |
| C24 | 0.3204 (9) | 0.2070 (4) | 0.8840 (9) | 0.126 (3) |
| H24 | 0.3032 | 0.2030 | 0.9536 | 0.151* |
| C25 | 0.2452 (9) | 0.1769 (3) | 0.7868 (10) | 0.129 (3) |
| H25 | 0.1775 | 0.1533 | 0.7872 | 0.155* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.134 (6) | 0.049 (4) | 0.098 (5) | 0.006 (3) | 0.026 (4) | −0.002 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.060 (3) | 0.039 (3) | 0.067 (4) | 0.002 (2) | 0.011 (2) | 0.008 (3) |
| C3 | 0.068 (3) | 0.058 (2) | 0.067 (4) | 0.004 (2) | 0.009 (3) | 0.022 (3) |
| C4 | 0.054 (2) | 0.063 (2) | 0.046 (2) | 0.003 (2) | 0.010 (2) | 0.012 (2) |
| C5 | 0.120 (5) | 0.093 (5) | 0.054 (3) | 0.018 (4) | 0.033 (3) | 0.010 (3) |
| C6 | 0.055 (2) | 0.049 (3) | 0.045 (3) | 0.0004 (19) | 0.013 (2) | −0.007 (2) |
| C7 | 0.046 (2) | 0.049 (3) | 0.041 (2) | 0.0039 (18) | 0.0108 (18) | −0.011 (2) |
| C8 | 0.060 (3) | 0.052 (3) | 0.065 (3) | 0.009 (2) | 0.019 (2) | 0.004 (3) |
| C9 | 0.047 (2) | 0.074 (4) | 0.081 (4) | 0.016 (2) | 0.016 (2) | 0.013 (3) |
| C10 | 0.044 (2) | 0.060 (3) | 0.065 (3) | 0.003 (2) | 0.016 (2) | −0.002 (3) |
| C11 | 0.045 (2) | 0.049 (3) | 0.039 (2) | 0.0046 (18) | 0.0148 (17) | −0.006 (2) |
| C12 | 0.0423 (19) | 0.048 (3) | 0.033 (2) | 0.0029 (17) | 0.0066 (16) | −0.006 (2) |
| C13 | 0.047 (2) | 0.055 (3) | 0.046 (3) | −0.0024 (19) | 0.0171 (19) | −0.006 (2) |
| C14 | 0.055 (3) | 0.091 (4) | 0.076 (4) | 0.001 (3) | 0.031 (3) | 0.012 (3) |
| C15 | 0.041 (2) | 0.054 (3) | 0.048 (3) | 0.0002 (19) | 0.0114 (18) | 0.008 (2) |
| C16 | 0.045 (2) | 0.051 (3) | 0.065 (3) | −0.0112 (19) | 0.006 (2) | 0.000 (3) |
| C17 | 0.047 (2) | 0.041 (3) | 0.051 (3) | −0.0023 (18) | 0.0063 (19) | −0.001 (2) |
| C18 | 0.077 (3) | 0.052 (3) | 0.059 (3) | −0.009 (2) | 0.011 (3) | −0.015 (3) |
| N1 | 0.0525 (19) | 0.038 (2) | 0.047 (2) | −0.0025 (15) | 0.0139 (16) | −0.0023 (18) |
| N2 | 0.0427 (17) | 0.047 (2) | 0.040 (2) | −0.0013 (15) | 0.0111 (15) | 0.0000 (18) |
| N3 | 0.0402 (16) | 0.043 (2) | 0.047 (2) | −0.0019 (14) | 0.0114 (15) | 0.0005 (17) |
| N4 | 0.0421 (16) | 0.041 (2) | 0.046 (2) | −0.0030 (14) | 0.0150 (15) | −0.0042 (17) |
| Cl1 | 0.0409 (5) | 0.0746 (9) | 0.0621 (8) | −0.0089 (5) | 0.0123 (5) | −0.0036 (6) |
| Cl2 | 0.0581 (6) | 0.0569 (8) | 0.0727 (9) | 0.0068 (5) | 0.0148 (6) | 0.0169 (7) |
| Cl3 | 0.0417 (5) | 0.0538 (7) | 0.0524 (7) | −0.0020 (4) | 0.0074 (4) | 0.0048 (5) |
| Cl4 | 0.0436 (5) | 0.0561 (7) | 0.0845 (9) | 0.0107 (5) | 0.0286 (5) | 0.0119 (7) |
| Pd1 | 0.03703 (15) | 0.0461 (2) | 0.04121 (19) | 0.00065 (13) | 0.01216 (13) | 0.00031 (16) |
| Pd2 | 0.03750 (15) | 0.03964 (19) | 0.0467 (2) | 0.00144 (12) | 0.01255 (13) | −0.00171 (15) |
| C19 | 0.199 (12) | 0.186 (12) | 0.217 (13) | 0.093 (10) | −0.019 (10) | −0.040 (11) |
| C20 | 0.126 (7) | 0.115 (7) | 0.167 (9) | 0.043 (5) | 0.056 (6) | 0.040 (7) |
| C21 | 0.153 (9) | 0.128 (9) | 0.208 (11) | 0.062 (5) | 0.122 (9) | 0.070 (7) |
| C22 | 0.174 (11) | 0.131 (9) | 0.249 (14) | 0.052 (7) | 0.145 (11) | 0.050 (8) |
| C23 | 0.118 (6) | 0.126 (7) | 0.220 (11) | 0.052 (4) | 0.082 (7) | 0.070 (8) |
| C24 | 0.115 (6) | 0.116 (7) | 0.167 (8) | 0.061 (4) | 0.076 (6) | 0.075 (6) |
| C25 | 0.116 (6) | 0.091 (6) | 0.187 (9) | 0.054 (5) | 0.065 (6) | 0.068 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.488 (8) | C15—N3 | 1.349 (5) |
| C1—H1A | 0.9600 | C15—C16 | 1.387 (6) |
| C1—H1B | 0.9600 | C16—C17 | 1.381 (7) |
| C1—H1C | 0.9600 | C16—H16 | 0.9300 |
| C2—N1 | 1.348 (6) | C17—N4 | 1.344 (5) |
| C2—C3 | 1.367 (7) | C17—C18 | 1.506 (7) |
| C3—C4 | 1.403 (7) | C18—H18A | 0.9600 |
| C3—H3 | 0.9300 | C18—H18B | 0.9600 |
| C4—N2 | 1.339 (6) | C18—H18C | 0.9600 |
| C4—C5 | 1.468 (7) | N1—N2 | 1.361 (5) |
| C5—H5A | 0.9600 | N2—Pd1 | 2.005 (3) |

| | | | |
|---|---|---|---|
| C5—H5B | 0.9600 | N3—N4 | 1.356 (5) |
| C5—H5C | 0.9600 | N4—Pd2 | 2.002 (3) |
| C6—N1 | 1.462 (6) | Cl1—Pd1 | 2.2647 (11) |
| C6—C7 | 1.524 (6) | Cl2—Pd2 | 2.2774 (12) |
| C6—H6A | 0.9700 | Cl3—Pd2 | 2.3421 (11) |
| C6—H6B | 0.9700 | Cl3—Pd1 | 2.3502 (10) |
| C7—C12 | 1.367 (6) | Cl4—Pd2 | 2.3092 (11) |
| C7—C8 | 1.402 (6) | Cl4—Pd1 | 2.3135 (12) |
| C8—C9 | 1.375 (7) | Pd1—Pd2 | 3.2117 (5) |
| C8—H8 | 0.9300 | C19—C20 | 1.435 (11) |
| C9—C10 | 1.371 (7) | C19—H19A | 0.9600 |
| C9—H9 | 0.9300 | C19—H19B | 0.9600 |
| C10—C11 | 1.393 (6) | C19—H19C | 0.9600 |
| C10—H10 | 0.9300 | C20—C21 | 1.341 (13) |
| C11—C12 | 1.393 (6) | C20—C25 | 1.391 (13) |
| C11—C13 | 1.511 (6) | C21—C22 | 1.435 (15) |
| C12—H12 | 0.9300 | C21—H21 | 0.9300 |
| C13—N3 | 1.474 (5) | C22—C23 | 1.292 (13) |
| C13—H13A | 0.9700 | C22—H22 | 0.9300 |
| C13—H13B | 0.9700 | C23—C24 | 1.418 (12) |
| C14—C15 | 1.484 (7) | C23—H23 | 0.9300 |
| C14—H14A | 0.9600 | C24—C25 | 1.370 (12) |
| C14—H14B | 0.9600 | C24—H24 | 0.9300 |
| C14—H14C | 0.9600 | C25—H25 | 0.9300 |

| | | | |
|---|---|---|---|
| C2—C1—H1A | 109.5 | C16—C17—C18 | 131.1 (4) |
| C2—C1—H1B | 109.5 | C17—C18—H18A | 109.5 |
| H1A—C1—H1B | 109.5 | C17—C18—H18B | 109.5 |
| C2—C1—H1C | 109.5 | H18A—C18—H18B | 109.5 |
| H1A—C1—H1C | 109.5 | C17—C18—H18C | 109.5 |
| H1B—C1—H1C | 109.5 | H18A—C18—H18C | 109.5 |
| N1—C2—C3 | 106.9 (4) | H18B—C18—H18C | 109.5 |
| N1—C2—C1 | 122.6 (5) | C2—N1—N2 | 110.1 (4) |
| C3—C2—C1 | 130.5 (5) | C2—N1—C6 | 129.4 (4) |
| C2—C3—C4 | 107.6 (5) | N2—N1—C6 | 120.0 (3) |
| C2—C3—H3 | 126.2 | C4—N2—N1 | 107.8 (4) |
| C4—C3—H3 | 126.2 | C4—N2—Pd1 | 127.2 (3) |
| N2—C4—C3 | 107.6 (5) | N1—N2—Pd1 | 122.3 (3) |
| N2—C4—C5 | 122.0 (5) | C15—N3—N4 | 111.1 (3) |
| C3—C4—C5 | 130.5 (5) | C15—N3—C13 | 128.9 (4) |
| C4—C5—H5A | 109.5 | N4—N3—C13 | 119.6 (3) |
| C4—C5—H5B | 109.5 | C17—N4—N3 | 106.8 (3) |
| H5A—C5—H5B | 109.5 | C17—N4—Pd2 | 126.8 (3) |
| C4—C5—H5C | 109.5 | N3—N4—Pd2 | 125.3 (2) |
| H5A—C5—H5C | 109.5 | Pd2—Cl3—Pd1 | 86.39 (3) |
| H5B—C5—H5C | 109.5 | Pd2—Cl4—Pd1 | 88.01 (4) |
| N1—C6—C7 | 111.6 (3) | N2—Pd1—Cl1 | 87.88 (10) |
| N1—C6—H6A | 109.3 | N2—Pd1—Cl4 | 178.57 (11) |

| | | | |
|---|---|---|---|
| C7—C6—H6A | 109.3 | Cl1—Pd1—Cl4 | 92.05 (4) |
| N1—C6—H6B | 109.3 | N2—Pd1—Cl3 | 94.55 (9) |
| C7—C6—H6B | 109.3 | Cl1—Pd1—Cl3 | 177.47 (5) |
| H6A—C6—H6B | 108.0 | Cl4—Pd1—Cl3 | 85.54 (4) |
| C12—C7—C8 | 119.7 (4) | N2—Pd1—Pd2 | 133.45 (9) |
| C12—C7—C6 | 120.3 (4) | Cl1—Pd1—Pd2 | 131.49 (4) |
| C8—C7—C6 | 120.0 (4) | Cl4—Pd1—Pd2 | 45.94 (3) |
| C9—C8—C7 | 119.3 (5) | Cl3—Pd1—Pd2 | 46.70 (3) |
| C9—C8—H8 | 120.4 | N4—Pd2—Cl2 | 89.80 (10) |
| C7—C8—H8 | 120.4 | N4—Pd2—Cl4 | 178.19 (11) |
| C10—C9—C8 | 120.9 (4) | Cl2—Pd2—Cl4 | 91.61 (4) |
| C10—C9—H9 | 119.6 | N4—Pd2—Cl3 | 92.76 (10) |
| C8—C9—H9 | 119.6 | Cl2—Pd2—Cl3 | 177.44 (4) |
| C9—C10—C11 | 120.5 (4) | Cl4—Pd2—Cl3 | 85.82 (4) |
| C9—C10—H10 | 119.7 | N4—Pd2—Pd1 | 133.22 (10) |
| C11—C10—H10 | 119.7 | Cl2—Pd2—Pd1 | 130.78 (3) |
| C12—C11—C10 | 118.4 (4) | Cl4—Pd2—Pd1 | 46.05 (3) |
| C12—C11—C13 | 120.8 (4) | Cl3—Pd2—Pd1 | 46.91 (3) |
| C10—C11—C13 | 120.8 (4) | C20—C19—H19A | 109.5 |
| C7—C12—C11 | 121.3 (4) | C20—C19—H19B | 109.5 |
| C7—C12—H12 | 119.4 | H19A—C19—H19B | 109.5 |
| C11—C12—H12 | 119.4 | C20—C19—H19C | 109.5 |
| N3—C13—C11 | 111.3 (3) | H19A—C19—H19C | 109.5 |
| N3—C13—H13A | 109.4 | H19B—C19—H19C | 109.5 |
| C11—C13—H13A | 109.4 | C21—C20—C19 | 121.7 (13) |
| N3—C13—H13B | 109.4 | C21—C20—C25 | 124.1 (12) |
| C11—C13—H13B | 109.4 | C19—C20—C25 | 114.2 (12) |
| H13A—C13—H13B | 108.0 | C20—C21—C22 | 118.4 (12) |
| C15—C14—H14A | 109.5 | C20—C21—H21 | 120.8 |
| C15—C14—H14B | 109.5 | C22—C21—H21 | 120.8 |
| H14A—C14—H14B | 109.5 | C23—C22—C21 | 120.7 (13) |
| C15—C14—H14C | 109.5 | C23—C22—H22 | 119.6 |
| H14A—C14—H14C | 109.5 | C21—C22—H22 | 119.6 |
| H14B—C14—H14C | 109.5 | C22—C23—C24 | 118.5 (13) |
| N3—C15—C16 | 105.8 (4) | C22—C23—H23 | 120.7 |
| N3—C15—C14 | 124.2 (4) | C24—C23—H23 | 120.7 |
| C16—C15—C14 | 130.1 (4) | C25—C24—C23 | 124.3 (11) |
| C17—C16—C15 | 107.4 (4) | C25—C24—H24 | 117.9 |
| C17—C16—H16 | 126.3 | C23—C24—H24 | 117.9 |
| C15—C16—H16 | 126.3 | C24—C25—C20 | 113.9 (10) |
| N4—C17—C16 | 108.9 (4) | C24—C25—H25 | 123.0 |
| N4—C17—C18 | 120.0 (4) | C20—C25—H25 | 123.0 |

| | | | |
|---|---|---|---|
| N1—C2—C3—C4 | 0.3 (5) | C15—N3—N4—C17 | 0.9 (5) |
| C1—C2—C3—C4 | 179.3 (5) | C13—N3—N4—C17 | 175.2 (3) |
| C2—C3—C4—N2 | −1.5 (5) | C15—N3—N4—Pd2 | 169.8 (3) |
| C2—C3—C4—C5 | 179.3 (5) | C13—N3—N4—Pd2 | −15.8 (5) |
| N1—C6—C7—C12 | −129.2 (4) | C4—N2—Pd1—Cl1 | −88.8 (3) |

| | | | |
|---|---|---|---|
| N1—C6—C7—C8 | 49.6 (6) | N1—N2—Pd1—Cl1 | 70.3 (3) |
| C12—C7—C8—C9 | −0.7 (7) | C4—N2—Pd1—Cl3 | 90.5 (3) |
| C6—C7—C8—C9 | −179.5 (5) | N1—N2—Pd1—Cl3 | −110.3 (3) |
| C7—C8—C9—C10 | 1.0 (8) | C4—N2—Pd1—Pd2 | 119.8 (3) |
| C8—C9—C10—C11 | 0.0 (8) | N1—N2—Pd1—Pd2 | −81.1 (3) |
| C9—C10—C11—C12 | −1.2 (7) | Pd2—Cl4—Pd1—Cl1 | −152.62 (5) |
| C9—C10—C11—C13 | 177.1 (4) | Pd2—Cl4—Pd1—Cl3 | 28.14 (4) |
| C8—C7—C12—C11 | −0.6 (6) | Pd2—Cl3—Pd1—N2 | 150.81 (11) |
| C6—C7—C12—C11 | 178.2 (4) | Pd2—Cl3—Pd1—Cl4 | −27.75 (4) |
| C10—C11—C12—C7 | 1.5 (6) | C17—N4—Pd2—Cl2 | 94.0 (4) |
| C13—C11—C12—C7 | −176.8 (4) | N3—N4—Pd2—Cl2 | −72.8 (3) |
| C12—C11—C13—N3 | 125.1 (4) | C17—N4—Pd2—Cl3 | −86.0 (3) |
| C10—C11—C13—N3 | −53.2 (5) | N3—N4—Pd2—Cl3 | 107.2 (3) |
| N3—C15—C16—C17 | 0.9 (5) | C17—N4—Pd2—Pd1 | −112.8 (3) |
| C14—C15—C16—C17 | −178.7 (5) | N3—N4—Pd2—Pd1 | 80.5 (3) |
| C15—C16—C17—N4 | −0.4 (5) | Pd1—Cl4—Pd2—Cl2 | 151.71 (5) |
| C15—C16—C17—C18 | 178.1 (5) | Pd1—Cl4—Pd2—Cl3 | −28.24 (4) |
| C3—C2—N1—N2 | 0.9 (5) | Pd1—Cl3—Pd2—N4 | −153.33 (10) |
| C1—C2—N1—N2 | −178.2 (5) | Pd1—Cl3—Pd2—Cl4 | 27.80 (4) |
| C3—C2—N1—C6 | 172.8 (4) | N2—Pd1—Pd2—N4 | −4.1 (2) |
| C1—C2—N1—C6 | −6.3 (7) | Cl1—Pd1—Pd2—N4 | −144.43 (15) |
| C7—C6—N1—C2 | −107.5 (5) | Cl4—Pd1—Pd2—N4 | 177.72 (15) |
| C7—C6—N1—N2 | 63.6 (5) | Cl3—Pd1—Pd2—N4 | 37.97 (14) |
| C3—C4—N2—N1 | 2.0 (5) | N2—Pd1—Pd2—Cl2 | 139.48 (15) |
| C5—C4—N2—N1 | −178.7 (4) | Cl1—Pd1—Pd2—Cl2 | −0.88 (7) |
| C3—C4—N2—Pd1 | 163.6 (3) | Cl4—Pd1—Pd2—Cl2 | −38.73 (7) |
| C5—C4—N2—Pd1 | −17.1 (6) | Cl3—Pd1—Pd2—Cl2 | −178.48 (7) |
| C2—N1—N2—C4 | −1.9 (4) | N2—Pd1—Pd2—Cl4 | 178.21 (15) |
| C6—N1—N2—C4 | −174.6 (3) | Cl1—Pd1—Pd2—Cl4 | 37.85 (7) |
| C2—N1—N2—Pd1 | −164.5 (3) | Cl3—Pd1—Pd2—Cl4 | −139.75 (6) |
| C6—N1—N2—Pd1 | 22.7 (4) | N2—Pd1—Pd2—Cl3 | −42.04 (14) |
| C16—C15—N3—N4 | −1.1 (5) | Cl1—Pd1—Pd2—Cl3 | 177.61 (6) |
| C14—C15—N3—N4 | 178.5 (4) | Cl4—Pd1—Pd2—Cl3 | 139.75 (7) |
| C16—C15—N3—C13 | −174.8 (4) | C19—C20—C21—C22 | −178.1 (9) |
| C14—C15—N3—C13 | 4.9 (7) | C25—C20—C21—C22 | 0.3 (14) |
| C11—C13—N3—C15 | 105.7 (5) | C20—C21—C22—C23 | 0.0 (16) |
| C11—C13—N3—N4 | −67.5 (4) | C21—C22—C23—C24 | 0.1 (15) |
| C16—C17—N4—N3 | −0.3 (5) | C22—C23—C24—C25 | −0.6 (13) |
| C18—C17—N4—N3 | −178.9 (4) | C23—C24—C25—C20 | 0.9 (12) |
| C16—C17—N4—Pd2 | −169.0 (3) | C21—C20—C25—C24 | −0.8 (12) |
| C18—C17—N4—Pd2 | 12.3 (6) | C19—C20—C25—C24 | 177.8 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16···*Cg*1$^{i}$ | 0.93 | 2.93 | 3.802 (6) | 157 |

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