

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

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

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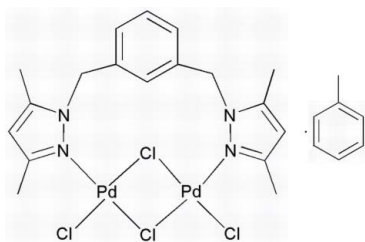
Received 17 March 2009; accepted 23 March 2009

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

In the title complex,  $[\text{Pd}_2\text{Cl}_4(\text{C}_{18}\text{H}_{22}\text{N}_4)] \cdot \text{C}_7\text{H}_8$ , each of the two four-coordinated  $\text{Pd}^{\text{II}}$  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  $\text{C}-\text{H} \cdots \pi$  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

 $[\text{Pd}_2\text{Cl}_4(\text{C}_{18}\text{H}_{22}\text{N}_4)] \cdot \text{C}_7\text{H}_8$  $M_r = 741.13$ 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<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 1.60$  mm<sup>-1</sup> $T = 298$  K $0.50 \times 0.12 \times 0.06$  mm

Absorption correction: multi-scan (SADABS; Bruker, 2001)

 $T_{\text{min}} = 0.503$ ,  $T_{\text{max}} = 0.910$ 22587 measured reflections  
7158 independent reflections4777 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$ 

### 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

 $\Delta\rho_{\text{max}} = 0.53$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.58$  e Å<sup>-3</sup>

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, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
Cl16—H16 $\cdots$ Cg1 <sup>1</sup>	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).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m446 [ doi:10.1107/S1600536809010629 ]

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

**B. Omondi, A. Budhai and J. Darkwa**

**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<sub>2</sub>X<sub>4</sub> (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<sub>2</sub> 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<sup>II</sup> 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 structures 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⋯ $\pi$  interaction, with an H16⋯ $\pi$  distance of 2.93 Å (Fig. 2).

**Experimental**

To a solution of PdCl<sub>2</sub>(NCMe)<sub>2</sub> (0.44 g, 1.70 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (25 mL) was added 1,3-bis[(3,5-dimethylpyrazole-1-yl)methyl]benzene (0.50 g, 1.70 mmol). The resultant solution was stirred overnight, and after removal of solvent, a dark orange solid was obtained. Recrystallization was done in a mixture of CHCl<sub>3</sub> and toluene, giving needle-shaped crystals.

## Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.97 (CH<sub>2</sub>) and 0.96 (CH<sub>3</sub>) Å and with  $U_{\text{iso}}(\text{H}) = 1.2$  (or 1.5 for methyl)  $U_{\text{eq}}(\text{C})$ .

## Figures

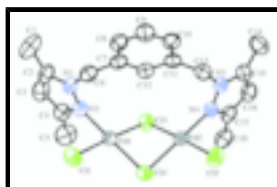


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms and toluene molecule have been omitted for clarity.

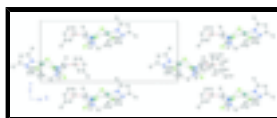


Fig. 2. Packing diagram of the title compound, showing the intermolecular C—H... $\pi$  interactions (dashed lines) linking the Pd complex and the toluene solvent molecule. [Symmetry code: (i)  $1/2+x, 3/2-y, -1/2+z$ .]

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### Crystal data

[Pd<sub>2</sub>Cl<sub>4</sub>(C<sub>18</sub>H<sub>22</sub>N<sub>4</sub>)]·C<sub>7</sub>H<sub>8</sub>

$M_r = 741.13$

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<sup>3</sup>

$Z = 4$

$F_{000} = 1472$

$D_x = 1.661$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 22587 reflections

$\theta = 2.0$ – $28.0$ °

$\mu = 1.60$  mm<sup>-1</sup>

$T = 298$  K

Needle, brown

$0.50 \times 0.12 \times 0.06$  mm

### Data collection

Bruker SMART APEX CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$  K

$\phi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\text{min}} = 0.503$ ,  $T_{\text{max}} = 0.910$

22587 measured reflections

7158 independent reflections

4777 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\text{max}} = 28.0$ °

$\theta_{\text{min}} = 2.0$ °

$h = -13 \rightarrow 13$

$k = -24 \rightarrow 33$

$l = -10 \rightarrow 15$

Refinement

Refinement on $F^2$	10 restraints
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 1.0406P]$
$wR(F^2) = 0.098$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\max} = 0.012$
7158 reflections	$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
321 parameters	$\Delta\rho_{\min} = -0.57 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

## supplementary materials

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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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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)
C11	0.0409 (5)	0.0746 (9)	0.0621 (8)	-0.0089 (5)	0.0123 (5)	-0.0036 (6)
C12	0.0581 (6)	0.0569 (8)	0.0727 (9)	0.0068 (5)	0.0148 (6)	0.0169 (7)
C13	0.0417 (5)	0.0538 (7)	0.0524 (7)	-0.0020 (4)	0.0074 (4)	0.0048 (5)
C14	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, °)*

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)	C11—Pd1	2.2647 (11)
C6—C7	1.524 (6)	C12—Pd2	2.2774 (12)
C6—H6A	0.9700	C13—Pd2	2.3421 (11)
C6—H6B	0.9700	C13—Pd1	2.3502 (10)
C7—C12	1.367 (6)	C14—Pd2	2.3092 (11)
C7—C8	1.402 (6)	C14—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

## supplementary materials

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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)	C14—Pd2—C13	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)	C14—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—C11	-88.8 (3)
N1—C6—C7—C8	49.6 (6)	N1—N2—Pd1—C11	70.3 (3)
C12—C7—C8—C9	-0.7 (7)	C4—N2—Pd1—C13	90.5 (3)
C6—C7—C8—C9	-179.5 (5)	N1—N2—Pd1—C13	-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—C11	-152.62 (5)
C9—C10—C11—C13	177.1 (4)	Pd2—Cl4—Pd1—C13	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—C14	-27.75 (4)
C10—C11—C12—C7	1.5 (6)	C17—N4—Pd2—C12	94.0 (4)
C13—C11—C12—C7	-176.8 (4)	N3—N4—Pd2—C12	-72.8 (3)
C12—C11—C13—N3	125.1 (4)	C17—N4—Pd2—C13	-86.0 (3)
C10—C11—C13—N3	-53.2 (5)	N3—N4—Pd2—C13	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)

## supplementary materials

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 ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16 $\cdots$ Cg1 <sup>i</sup>	0.93	2.93	3.802 (6)	157

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

Fig. 1

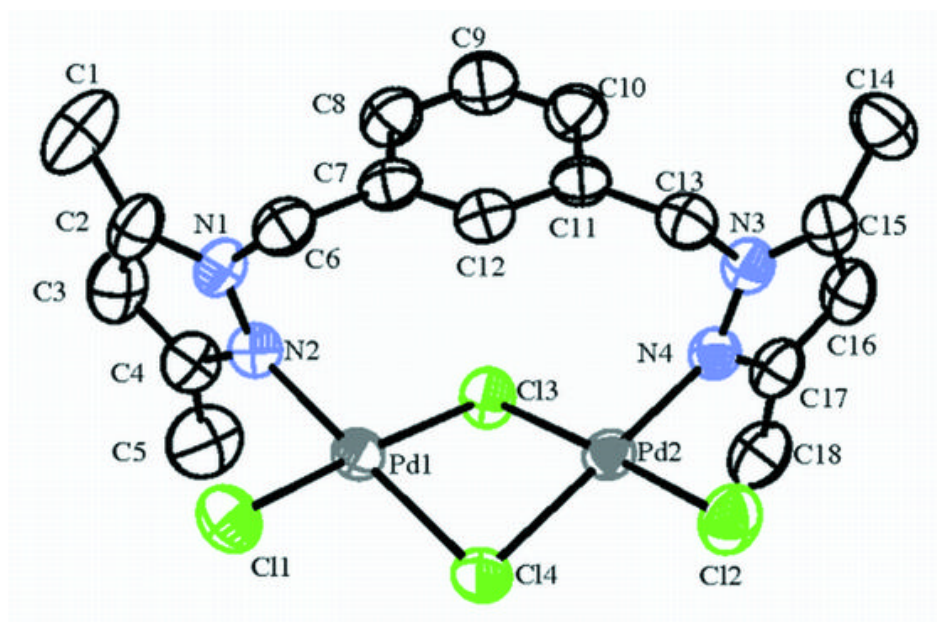


Fig. 2

