

## Di- $\mu$ -acetato- $\kappa^4$ O:O'-bis[[2-(2-pyridyl)-phenyl- $\kappa^2$ C,N]palladium(II)]

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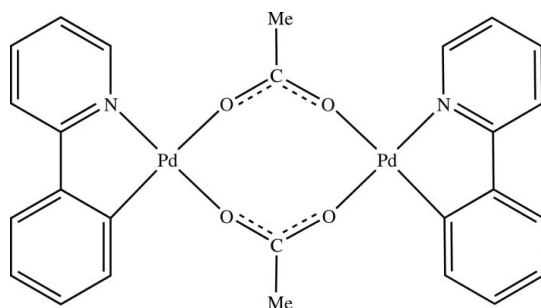
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.072; data-to-parameter ratio = 16.2.

In the title complex,  $[\text{Pd}_2(\text{C}_{11}\text{H}_8\text{N})_2(\text{C}_2\text{H}_3\text{O}_2)_2]$ , each  $\text{Pd}^{\text{II}}$  ion has a distorted square-planar environment, being surrounded by one C, one N and two O atoms. The  $\text{Pd}\cdots\text{Pd}$  distance is 2.8721 (3) Å. In the crystal structure, the molecules are linked by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions.

### Related literature

For related compounds, see: Cravotto *et al.* (2005). For the synthesis, see: Aiello *et al.* (2000). For background information on graph-set theory, see: Bernstein *et al.* (1995).



### Experimental

#### Crystal data

$[\text{Pd}_2(\text{C}_{11}\text{H}_8\text{N})_2(\text{C}_2\text{H}_3\text{O}_2)_2]$

$M_r = 639.26$

Monoclinic,  $P2_1/c$

$a = 9.7160$  (3) Å

$b = 19.1986$  (5) Å

$c = 14.4990$  (4) Å

$\beta = 119.451$  (2)°

$V = 2355.06$  (12) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 1.56$  mm<sup>-1</sup>

$T = 296$  K

$0.46 \times 0.31 \times 0.22$  mm

#### Data collection

Stoe IPDSII diffractometer

Absorption correction: integration

(*X-RED*; Stoe & Cie, 2002)

$T_{\text{min}} = 0.355$ ,  $T_{\text{max}} = 0.728$

23605 measured reflections

5011 independent reflections

4375 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.136$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.071$

$S = 1.05$

5011 reflections

309 parameters

2 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.77$  e Å<sup>-3</sup>

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

Table 1

Selected bond lengths (Å).

Pd1—C11	1.960 (3)	Pd2—N2	1.961 (3)
Pd1—N1	2.006 (2)	Pd2—C24	2.002 (3)
Pd1—O2	2.052 (2)	Pd2—O3	2.058 (2)
Pd1—O1	2.143 (2)	Pd2—O4	2.155 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 $\cdots$ O1	0.93	2.56	3.134 (4)	120
C23—H23 $\cdots$ O4	0.93	2.57	3.146 (4)	120
C14—H14 $\cdots$ O3	0.93	2.54	3.054 (5)	115
C10—H10 $\cdots$ O2	0.93	2.56	3.069 (4)	115
C7—H7 $\cdots$ O3 <sup>i</sup>	0.93	2.56	3.344 (4)	142

Symmetry code: (i)  $x + 1, y, z$ .

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2692).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m381 [ doi:10.1107/S1600536808001736 ]

## Di- $\mu$ -acetato- $\kappa^4 O:O'$ -bis{[2-(2-pyridyl)phenyl- $\kappa^2 C,N$ ]palladium(II)}

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### Comment

Cyclometalated compounds are organometallic complexes embodying an E—M—C connectivity of  $\sigma$ -bonds, where E is a heterodonor atom of the 15- or 16-group, M is a metallic atom and C is a carbon donor. They are usually classified according to the metal, the donor atom(s) or chelate ring size. Cyclometalated compounds with a variety of N-donor ligands have been extensively investigated (Cravotto *et al.*, 2005).

The structure of the title dinuclear complex, (I), is shown in Fig. 1. The coordination around the Pd<sup>II</sup> ions is distorted square-planar, and each Pd<sup>II</sup> ion is coordinated by one pyridine N atom and one aryl C atom from the phenylpyridine ligand and two O atoms from two acetate ligands (Table 1). The pyridine N- and aryl C-donor atoms form two five-membered metallacycles (containing atoms N1/C5/C6/C11/Pd1 and N2/C18/C19/C24/Pd2) with maximum deviations from planarity being -0.033 (2) and 0.0399 (2) Å for atoms N1 and C24, respectively. The separation of the Pd centres in the molecule of (I) is a relatively short 2.8721 (3) Å.

Four short C—H $\cdots$ O intramolecular interactions (Table 2) are observed between the phenylpyridine H atoms and acetate O atoms, all of which lead to the formation of a five-membered ring with graph-set descriptor S(5) (Bernstein *et al.*, 1995). In the crystal structure of (I), an intermolecular C—H $\cdots$ O interaction involving an aryl C—H donor and acetate acceptor is seen. Propagation of this hydrogen bond by translation then generates a C(8) chain running parallel to the [100] direction (Fig. 2). There are no other significant directional interactions in the crystal of (I).

### Experimental

The title compound was synthesized according to a modification of literature methods (Aiello *et al.*, 2000) and colourless prisms of (I) were grown from CH<sub>2</sub>Cl<sub>2</sub>/hexane (1:3 v/v).

### Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The methyl groups were allowed to rotate, but not to tip, to best fit the electron density.

Figures

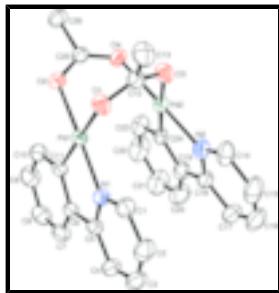


Fig. 1. A view of the molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

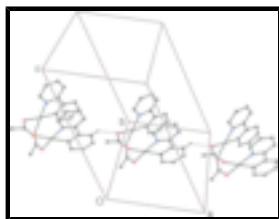


Fig. 2. Part of the crystal structure of (I), showing a C(8) chain along [100]. For the sake of clarity, only H atoms involved in hydrogen bonding have been included.

**Di- $\mu$ -acetato- $\kappa^4$ O:O'-bis{[2-(2-pyridyl)phenyl- $\kappa^2$ C,N]}palladium(II)}**

*Crystal data*

[Pd<sub>2</sub>(C<sub>11</sub>H<sub>8</sub>N)<sub>2</sub>(C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>)<sub>2</sub>]

$M_r = 639.26$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 9.7160$  (3) Å

$b = 19.1986$  (5) Å

$c = 14.4990$  (4) Å

$\beta = 119.451$  (2)°

$V = 2355.06$  (12) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1264$

$D_x = 1.803$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 33146 reflections

$\theta = 1.6$ – $27.3$ °

$\mu = 1.56$  mm<sup>-1</sup>

$T = 296$  K

Prism, colorless

$0.46 \times 0.31 \times 0.22$  mm

*Data collection*

Stoe IPDSII  
diffractometer

5011 independent reflections

Radiation source: sealed X-ray tube, 12 x 0.4 mm  
long-fine focus

4375 reflections with  $I > 2\sigma(I)$

Monochromator: plane graphite

$R_{int} = 0.136$

Detector resolution: 6.67 pixels mm<sup>-1</sup>

$\theta_{max} = 26.8$ °

$T = 296$  K

$\theta_{min} = 1.9$ °

$\omega$  scans

$h = -12 \rightarrow 12$

Absorption correction: integration  
(X-RED; Stoe & Cie, 2002)

$k = -24 \rightarrow 24$

$T_{min} = 0.355$ ,  $T_{max} = 0.728$

$l = -18 \rightarrow 18$

23605 measured reflections

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.5683P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
5011 reflections	$(\Delta/\sigma)_{\max} = 0.001$
309 parameters	$\Delta\rho_{\max} = 0.77 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd1	0.46714 (2)	0.310590 (12)	0.223710 (16)	0.04341 (7)
Pd2	0.37093 (2)	0.410977 (12)	0.327729 (17)	0.04429 (7)
O1	0.3311 (3)	0.24915 (12)	0.27333 (19)	0.0561 (5)
O2	0.2637 (2)	0.33997 (13)	0.09023 (16)	0.0557 (5)
O3	0.2400 (3)	0.33063 (12)	0.33927 (19)	0.0587 (5)
O4	0.1952 (2)	0.42585 (12)	0.16407 (17)	0.0578 (5)
N1	0.6762 (3)	0.28819 (13)	0.35073 (19)	0.0477 (5)
N2	0.5367 (4)	0.40253 (16)	0.4762 (2)	0.0630 (7)
C1	0.6946 (4)	0.25087 (19)	0.4345 (3)	0.0604 (8)
H1	0.6069	0.2296	0.4321	0.072*
C2	0.8396 (5)	0.2433 (2)	0.5233 (3)	0.0738 (10)
H2	0.8497	0.2178	0.5809	0.089*
C3	0.9692 (5)	0.2737 (2)	0.5265 (3)	0.0725 (10)
H3	1.0684	0.2688	0.5860	0.087*
C4	0.9516 (4)	0.31178 (19)	0.4409 (3)	0.0628 (9)
H4	1.0391	0.3324	0.4421	0.075*

## supplementary materials

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C5	0.8032 (3)	0.31928 (16)	0.3532 (2)	0.0483 (7)
C6	0.7649 (3)	0.35957 (16)	0.2578 (2)	0.0481 (6)
C7	0.8747 (4)	0.3950 (2)	0.2408 (3)	0.0626 (8)
H7	0.9813	0.3938	0.2915	0.075*
C8	0.8254 (5)	0.4318 (2)	0.1492 (4)	0.0744 (10)
H8	0.8987	0.4565	0.1384	0.089*
C9	0.6682 (5)	0.4327 (2)	0.0726 (3)	0.0735 (10)
H9	0.6363	0.4574	0.0101	0.088*
C10	0.5574 (4)	0.3970 (2)	0.0883 (3)	0.0608 (8)
H10	0.4515	0.3977	0.0362	0.073*
C11	0.6038 (3)	0.36020 (16)	0.1816 (2)	0.0458 (6)
C12	0.2494 (3)	0.26915 (17)	0.3132 (2)	0.0481 (6)
C13	0.1557 (5)	0.2155 (2)	0.3327 (3)	0.0698 (9)
H13A	0.0459	0.2281	0.2955	0.105*
H13B	0.1916	0.2128	0.4072	0.105*
H13C	0.1694	0.1710	0.3079	0.105*
C14	0.5364 (5)	0.35817 (19)	0.5515 (3)	0.0684 (9)
H14	0.4499	0.3295	0.5341	0.082*
C15	0.6653 (7)	0.3566 (3)	0.6527 (3)	0.0889 (14)
H15	0.6651	0.3266	0.7029	0.107*
C16	0.7926 (6)	0.3987 (3)	0.6796 (3)	0.0928 (15)
H16	0.8782	0.3970	0.7480	0.111*
C17	0.7961 (5)	0.4436 (2)	0.6071 (3)	0.0780 (11)
H17	0.8829	0.4724	0.6262	0.094*
C18	0.6680 (4)	0.44554 (18)	0.5045 (2)	0.0557 (7)
C19	0.6545 (4)	0.49149 (18)	0.4208 (3)	0.0573 (8)
C20	0.7699 (5)	0.5372 (3)	0.4277 (4)	0.0861 (12)
H20	0.8667	0.5403	0.4898	0.103*
C21	0.7393 (7)	0.5778 (3)	0.3416 (4)	0.1022 (17)
H21	0.8159	0.6083	0.3449	0.123*
C22	0.5970 (7)	0.5733 (3)	0.2518 (4)	0.0976 (15)
H22	0.5747	0.6014	0.1938	0.117*
C23	0.4870 (5)	0.5270 (2)	0.2474 (3)	0.0681 (9)
H23	0.3900	0.5237	0.1856	0.082*
C24	0.5157 (3)	0.48611 (14)	0.3303 (2)	0.0416 (5)
C25	0.1765 (3)	0.38936 (17)	0.0883 (2)	0.0474 (6)
C26	0.0362 (4)	0.4046 (2)	-0.0187 (3)	0.0638 (9)
H26A	0.0063	0.3631	-0.0611	0.096*
H26B	0.0635	0.4403	-0.0532	0.096*
H26C	-0.0506	0.4201	-0.0100	0.096*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pd1	0.03742 (11)	0.05360 (14)	0.03992 (12)	0.00322 (8)	0.01957 (9)	0.00016 (9)
Pd2	0.04767 (12)	0.04564 (13)	0.03768 (12)	-0.00157 (9)	0.01955 (9)	-0.00403 (8)
O1	0.0602 (12)	0.0562 (13)	0.0631 (14)	-0.0076 (10)	0.0389 (11)	-0.0048 (10)
O2	0.0432 (10)	0.0747 (15)	0.0419 (11)	0.0066 (10)	0.0152 (9)	-0.0035 (10)

O3	0.0604 (12)	0.0579 (14)	0.0684 (14)	-0.0080 (10)	0.0398 (12)	-0.0069 (11)
O4	0.0537 (11)	0.0646 (14)	0.0418 (11)	0.0053 (10)	0.0132 (9)	-0.0057 (10)
N1	0.0469 (12)	0.0501 (14)	0.0432 (13)	0.0082 (10)	0.0199 (10)	0.0013 (10)
N2	0.0736 (17)	0.0631 (18)	0.0487 (15)	0.0099 (13)	0.0274 (14)	-0.0043 (12)
C1	0.0651 (19)	0.063 (2)	0.0504 (18)	0.0116 (16)	0.0263 (15)	0.0092 (15)
C2	0.090 (3)	0.066 (2)	0.051 (2)	0.020 (2)	0.0230 (19)	0.0106 (17)
C3	0.065 (2)	0.071 (2)	0.053 (2)	0.0180 (18)	0.0063 (16)	-0.0018 (17)
C4	0.0477 (16)	0.068 (2)	0.0557 (19)	0.0065 (14)	0.0123 (14)	-0.0086 (16)
C5	0.0424 (13)	0.0499 (17)	0.0481 (16)	0.0068 (11)	0.0186 (12)	-0.0059 (12)
C6	0.0415 (13)	0.0537 (17)	0.0526 (16)	0.0023 (12)	0.0257 (12)	-0.0072 (13)
C7	0.0514 (16)	0.069 (2)	0.073 (2)	-0.0041 (15)	0.0350 (16)	-0.0075 (18)
C8	0.073 (2)	0.080 (3)	0.094 (3)	-0.0062 (19)	0.059 (2)	0.003 (2)
C9	0.088 (3)	0.079 (3)	0.072 (2)	0.006 (2)	0.053 (2)	0.018 (2)
C10	0.0582 (17)	0.076 (2)	0.0517 (18)	0.0060 (16)	0.0297 (15)	0.0098 (16)
C11	0.0439 (13)	0.0539 (17)	0.0433 (14)	0.0059 (12)	0.0242 (12)	-0.0004 (12)
C12	0.0460 (14)	0.0577 (19)	0.0417 (14)	-0.0087 (12)	0.0224 (12)	-0.0016 (13)
C13	0.081 (2)	0.068 (2)	0.079 (2)	-0.0179 (18)	0.054 (2)	-0.0039 (19)
C14	0.098 (3)	0.058 (2)	0.0485 (18)	0.0091 (18)	0.0361 (18)	0.0047 (15)
C15	0.128 (4)	0.081 (3)	0.048 (2)	0.032 (3)	0.036 (2)	0.0149 (19)
C16	0.099 (3)	0.103 (4)	0.043 (2)	0.033 (3)	0.010 (2)	0.001 (2)
C17	0.062 (2)	0.094 (3)	0.053 (2)	0.0101 (19)	0.0091 (17)	-0.014 (2)
C18	0.0552 (16)	0.0581 (19)	0.0430 (15)	0.0067 (13)	0.0158 (13)	-0.0094 (14)
C19	0.0600 (17)	0.0573 (19)	0.0545 (18)	-0.0082 (14)	0.0280 (15)	-0.0130 (15)
C20	0.076 (2)	0.095 (3)	0.080 (3)	-0.032 (2)	0.032 (2)	-0.022 (2)
C21	0.113 (4)	0.108 (4)	0.094 (4)	-0.057 (3)	0.057 (3)	-0.016 (3)
C22	0.135 (4)	0.085 (3)	0.080 (3)	-0.041 (3)	0.058 (3)	-0.004 (2)
C23	0.084 (2)	0.060 (2)	0.0573 (19)	-0.0155 (18)	0.0328 (18)	-0.0033 (15)
C24	0.0495 (14)	0.0367 (13)	0.0384 (13)	-0.0045 (11)	0.0214 (11)	-0.0059 (10)
C25	0.0419 (13)	0.0567 (17)	0.0392 (14)	-0.0024 (12)	0.0166 (11)	0.0028 (12)
C26	0.0583 (18)	0.073 (2)	0.0446 (17)	0.0090 (16)	0.0130 (14)	0.0026 (15)

*Geometric parameters (Å, °)*

Pd1—C11	1.960 (3)	C9—C10	1.387 (5)
Pd1—N1	2.006 (2)	C9—H9	0.9300
Pd1—O2	2.052 (2)	C10—C11	1.390 (4)
Pd1—O1	2.143 (2)	C10—H10	0.9300
Pd1—Pd2	2.8721 (3)	C12—C13	1.491 (4)
Pd2—N2	1.961 (3)	C13—H13A	0.9600
Pd2—C24	2.002 (3)	C13—H13B	0.9600
Pd2—O3	2.058 (2)	C13—H13C	0.9600
Pd2—O4	2.155 (2)	C14—C15	1.384 (6)
O1—C12	1.250 (4)	C14—H14	0.9300
O2—C25	1.262 (4)	C15—C16	1.364 (7)
O3—C12	1.256 (4)	C15—H15	0.9300
O4—C25	1.239 (4)	C16—C17	1.372 (7)
N1—C1	1.344 (4)	C16—H16	0.9300
N1—C5	1.356 (4)	C17—C18	1.394 (5)
N2—C14	1.386 (5)	C17—H17	0.9300

## supplementary materials

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N2—C18	1.401 (5)	C18—C19	1.453 (5)
C1—C2	1.371 (5)	C19—C24	1.346 (4)
C1—H1	0.9300	C19—C20	1.388 (5)
C2—C3	1.368 (6)	C20—C21	1.374 (7)
C2—H2	0.9300	C20—H20	0.9300
C3—C4	1.376 (6)	C21—C22	1.358 (7)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.384 (4)	C22—C23	1.367 (6)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.464 (4)	C23—C24	1.345 (5)
C6—C7	1.386 (4)	C23—H23	0.9300
C6—C11	1.404 (4)	C25—C26	1.507 (4)
C7—C8	1.367 (6)	C26—H26A	0.9600
C7—H7	0.9300	C26—H26B	0.9600
C8—C9	1.377 (6)	C26—H26C	0.9600
C8—H8	0.9300		
C11—Pd1—N1	81.67 (11)	C9—C10—C11	120.3 (3)
C11—Pd1—O2	93.36 (10)	C9—C10—H10	119.8
N1—Pd1—O2	174.91 (10)	C11—C10—H10	119.8
C11—Pd1—O1	175.22 (10)	C10—C11—C6	118.2 (3)
N1—Pd1—O1	94.99 (10)	C10—C11—Pd1	127.2 (2)
O2—Pd1—O1	90.03 (9)	C6—C11—Pd1	114.5 (2)
C11—Pd1—Pd2	106.43 (9)	O1—C12—O3	125.7 (3)
N1—Pd1—Pd2	96.07 (7)	O1—C12—C13	117.4 (3)
O2—Pd1—Pd2	84.23 (6)	O3—C12—C13	116.8 (3)
O1—Pd1—Pd2	77.25 (6)	C12—C13—H13A	109.5
N2—Pd2—C24	81.30 (12)	C12—C13—H13B	109.5
N2—Pd2—O3	93.19 (12)	H13A—C13—H13B	109.5
C24—Pd2—O3	174.36 (10)	C12—C13—H13C	109.5
N2—Pd2—O4	176.64 (11)	H13A—C13—H13C	109.5
C24—Pd2—O4	95.39 (10)	H13B—C13—H13C	109.5
O3—Pd2—O4	90.13 (9)	C15—C14—N2	119.8 (4)
N2—Pd2—Pd1	102.55 (8)	C15—C14—H14	120.1
C24—Pd2—Pd1	94.94 (8)	N2—C14—H14	120.1
O3—Pd2—Pd1	85.04 (6)	C16—C15—C14	120.7 (4)
O4—Pd2—Pd1	78.28 (6)	C16—C15—H15	119.6
C12—O1—Pd1	128.5 (2)	C14—C15—H15	119.6
C25—O2—Pd1	123.52 (19)	C15—C16—C17	120.9 (4)
C12—O3—Pd2	122.73 (19)	C15—C16—H16	119.6
C25—O4—Pd2	126.4 (2)	C17—C16—H16	119.6
C1—N1—C5	119.7 (3)	C16—C17—C18	119.3 (4)
C1—N1—Pd1	124.7 (2)	C16—C17—H17	120.4
C5—N1—Pd1	115.3 (2)	C18—C17—H17	120.4
C14—N2—C18	119.0 (3)	C17—C18—N2	120.2 (4)
C14—N2—Pd2	126.7 (3)	C17—C18—C19	125.1 (4)
C18—N2—Pd2	114.3 (2)	N2—C18—C19	114.7 (3)
N1—C1—C2	121.6 (4)	C24—C19—C20	120.4 (4)
N1—C1—H1	119.2	C24—C19—C18	113.8 (3)
C2—C1—H1	119.2	C20—C19—C18	125.8 (3)

C3—C2—C1	119.4 (4)	C21—C20—C19	119.1 (4)
C3—C2—H2	120.3	C21—C20—H20	120.5
C1—C2—H2	120.3	C19—C20—H20	120.5
C2—C3—C4	119.5 (3)	C22—C21—C20	119.9 (4)
C2—C3—H3	120.3	C22—C21—H21	120.0
C4—C3—H3	120.3	C20—C21—H21	120.0
C3—C4—C5	119.7 (4)	C21—C22—C23	119.3 (4)
C3—C4—H4	120.1	C21—C22—H22	120.3
C5—C4—H4	120.1	C23—C22—H22	120.3
N1—C5—C4	120.1 (3)	C24—C23—C22	121.6 (4)
N1—C5—C6	113.7 (2)	C24—C23—H23	119.2
C4—C5—C6	126.2 (3)	C22—C23—H23	119.2
C7—C6—C11	120.9 (3)	C23—C24—C19	119.7 (3)
C7—C6—C5	124.5 (3)	C23—C24—Pd2	124.7 (2)
C11—C6—C5	114.6 (3)	C19—C24—Pd2	115.5 (2)
C8—C7—C6	119.6 (3)	O4—C25—O2	126.9 (3)
C8—C7—H7	120.2	O4—C25—C26	117.8 (3)
C6—C7—H7	120.2	O2—C25—C26	115.2 (3)
C7—C8—C9	120.7 (3)	C25—C26—H26A	109.5
C7—C8—H8	119.7	C25—C26—H26B	109.5
C9—C8—H8	119.7	H26A—C26—H26B	109.5
C8—C9—C10	120.2 (4)	C25—C26—H26C	109.5
C8—C9—H9	119.9	H26A—C26—H26C	109.5
C10—C9—H9	119.9	H26B—C26—H26C	109.5
C11—Pd1—Pd2—N2	-90.26 (13)	C5—C6—C7—C8	-179.2 (3)
N1—Pd1—Pd2—N2	-7.18 (12)	C6—C7—C8—C9	-1.4 (6)
O2—Pd1—Pd2—N2	177.93 (12)	C7—C8—C9—C10	0.9 (6)
O1—Pd1—Pd2—N2	86.58 (12)	C8—C9—C10—C11	0.2 (6)
C11—Pd1—Pd2—C24	-8.09 (11)	C9—C10—C11—C6	-0.8 (5)
N1—Pd1—Pd2—C24	74.99 (11)	C9—C10—C11—Pd1	176.4 (3)
O2—Pd1—Pd2—C24	-99.90 (10)	C7—C6—C11—C10	0.4 (5)
O1—Pd1—Pd2—C24	168.75 (10)	C5—C6—C11—C10	-179.7 (3)
C11—Pd1—Pd2—O3	177.57 (11)	C7—C6—C11—Pd1	-177.3 (2)
N1—Pd1—Pd2—O3	-99.35 (10)	C5—C6—C11—Pd1	2.7 (3)
O2—Pd1—Pd2—O3	85.76 (10)	N1—Pd1—C11—C10	178.7 (3)
O1—Pd1—Pd2—O3	-5.59 (9)	O2—Pd1—C11—C10	-2.4 (3)
C11—Pd1—Pd2—O4	86.40 (11)	Pd2—Pd1—C11—C10	-87.4 (3)
N1—Pd1—Pd2—O4	169.48 (10)	N1—Pd1—C11—C6	-3.9 (2)
O2—Pd1—Pd2—O4	-5.41 (9)	O2—Pd1—C11—C6	175.0 (2)
O1—Pd1—Pd2—O4	-96.75 (9)	Pd2—Pd1—C11—C6	90.0 (2)
N1—Pd1—O1—C12	102.8 (3)	Pd1—O1—C12—O3	-5.4 (5)
O2—Pd1—O1—C12	-76.3 (3)	Pd1—O1—C12—C13	175.2 (2)
Pd2—Pd1—O1—C12	7.7 (2)	Pd2—O3—C12—O1	-3.4 (4)
C11—Pd1—O2—C25	-100.1 (3)	Pd2—O3—C12—C13	176.0 (2)
O1—Pd1—O2—C25	83.3 (2)	C18—N2—C14—C15	-0.4 (5)
Pd2—Pd1—O2—C25	6.1 (2)	Pd2—N2—C14—C15	177.9 (3)
N2—Pd2—O3—C12	-95.5 (3)	N2—C14—C15—C16	0.4 (6)
O4—Pd2—O3—C12	85.1 (2)	C14—C15—C16—C17	0.0 (7)
Pd1—Pd2—O3—C12	6.8 (2)	C15—C16—C17—C18	-0.5 (7)

## supplementary materials

C24—Pd2—O4—C25	101.8 (3)	C16—C17—C18—N2	0.6 (6)
O3—Pd2—O4—C25	-77.1 (3)	C16—C17—C18—C19	178.5 (4)
Pd1—Pd2—O4—C25	7.8 (2)	C14—N2—C18—C17	-0.1 (5)
C11—Pd1—N1—C1	178.4 (3)	Pd2—N2—C18—C17	-178.6 (3)
O1—Pd1—N1—C1	-5.0 (3)	C14—N2—C18—C19	-178.3 (3)
Pd2—Pd1—N1—C1	72.7 (3)	Pd2—N2—C18—C19	3.3 (4)
C11—Pd1—N1—C5	4.7 (2)	C17—C18—C19—C24	-176.6 (3)
O1—Pd1—N1—C5	-178.8 (2)	N2—C18—C19—C24	1.4 (4)
Pd2—Pd1—N1—C5	-101.1 (2)	C17—C18—C19—C20	4.2 (6)
C24—Pd2—N2—C14	176.9 (3)	N2—C18—C19—C20	-177.7 (4)
O3—Pd2—N2—C14	-4.3 (3)	C24—C19—C20—C21	1.3 (7)
Pd1—Pd2—N2—C14	-89.9 (3)	C18—C19—C20—C21	-179.6 (4)
C24—Pd2—N2—C18	-4.7 (2)	C19—C20—C21—C22	0.6 (8)
O3—Pd2—N2—C18	174.0 (2)	C20—C21—C22—C23	-1.5 (9)
Pd1—Pd2—N2—C18	88.4 (2)	C21—C22—C23—C24	0.5 (8)
C5—N1—C1—C2	0.1 (5)	C22—C23—C24—C19	1.4 (6)
Pd1—N1—C1—C2	-173.4 (3)	C22—C23—C24—Pd2	-174.3 (3)
N1—C1—C2—C3	-0.9 (6)	C20—C19—C24—C23	-2.3 (5)
C1—C2—C3—C4	0.5 (6)	C18—C19—C24—C23	178.6 (3)
C2—C3—C4—C5	0.5 (5)	C20—C19—C24—Pd2	173.8 (3)
C1—N1—C5—C4	0.9 (4)	C18—C19—C24—Pd2	-5.4 (4)
Pd1—N1—C5—C4	175.0 (2)	N2—Pd2—C24—C23	-178.5 (3)
C1—N1—C5—C6	-178.5 (3)	O4—Pd2—C24—C23	0.9 (3)
Pd1—N1—C5—C6	-4.4 (3)	Pd1—Pd2—C24—C23	79.5 (3)
C3—C4—C5—N1	-1.2 (5)	N2—Pd2—C24—C19	5.7 (2)
C3—C4—C5—C6	178.1 (3)	O4—Pd2—C24—C19	-174.9 (2)
N1—C5—C6—C7	-178.9 (3)	Pd1—Pd2—C24—C19	-96.2 (2)
C4—C5—C6—C7	1.7 (5)	Pd2—O4—C25—O2	-6.2 (5)
N1—C5—C6—C11	1.1 (4)	Pd2—O4—C25—C26	174.2 (2)
C4—C5—C6—C11	-178.2 (3)	Pd1—O2—C25—O4	-2.2 (5)
C11—C6—C7—C8	0.8 (5)	Pd1—O2—C25—C26	177.4 (2)

### 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>
C1—H1...O1	0.93	2.56	3.134 (4)	120
C23—H23...O4	0.93	2.57	3.146 (4)	120
C14—H14...O3	0.93	2.54	3.054 (5)	115
C10—H10...O2	0.93	2.56	3.069 (4)	115
C7—H7...O3 <sup>i</sup>	0.93	2.56	3.344 (4)	142

Symmetry codes: (i)  $x+1, y, z$ .

Fig. 1

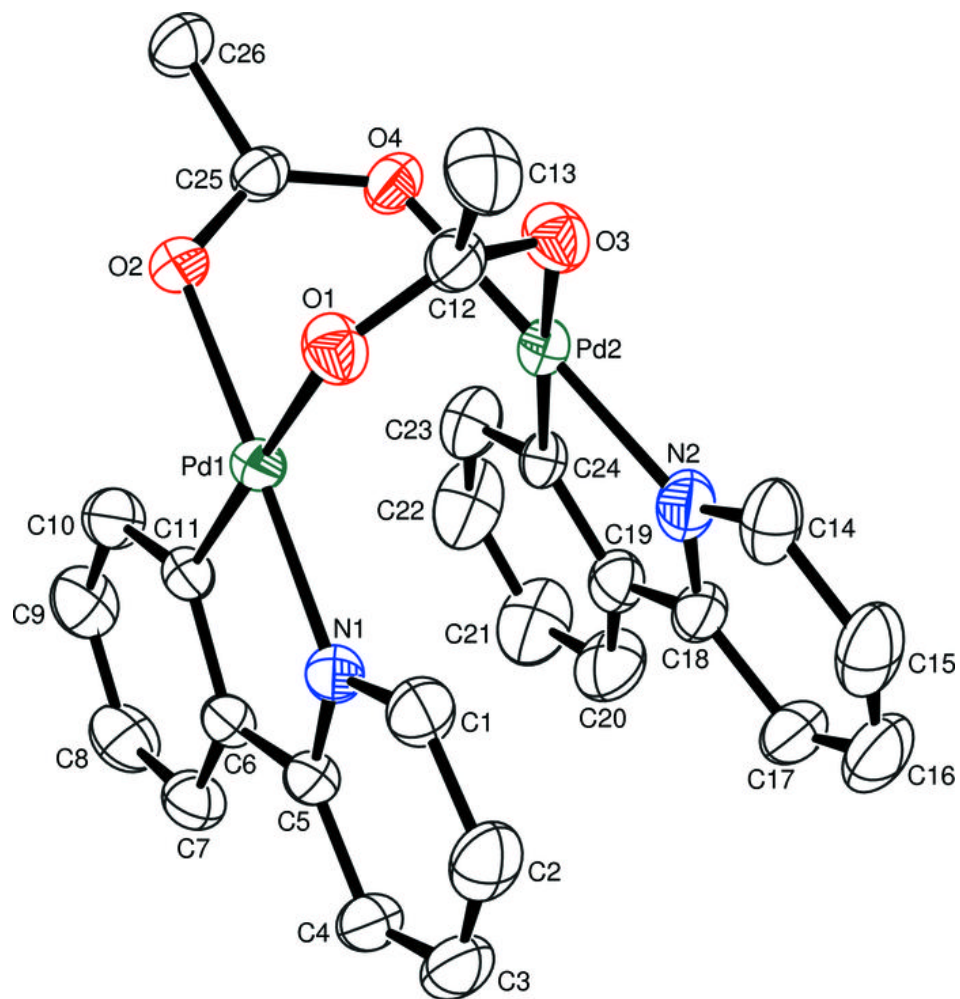


Fig. 2

