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(2,2′-Bipyridine-κ^2N,N')(pyridine-2,6-dicarboxylato-κ^2N,O)palladium(II) monohydrate

Kwang Ha*

Chonnam National University, School of Chemical Engineering, Research Institute of Catalysis, Gwangju, Republic of Korea. *Correspondence e-mail: hakwang@chonnam.ac.kr

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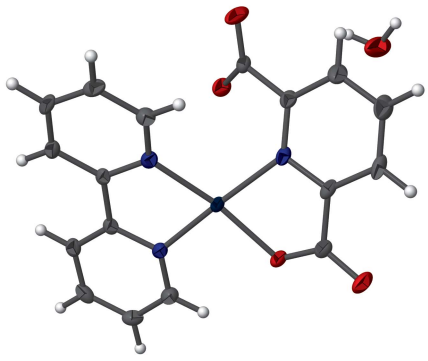
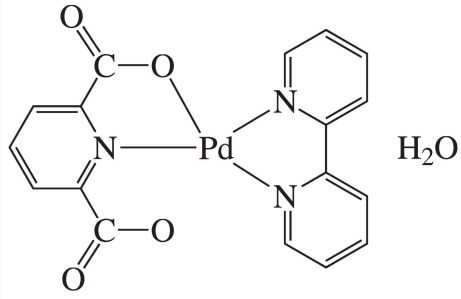
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$, the Pd^{II} cation is four-coordinated in a distorted square-planar coordination geometry defined by the two N atoms of the 2,2′-bipyridine ligand, one O atom and one N atom from the pyridine-2,6-dicarboxylate anion. The complex and solvent water molecule are linked by intermolecular hydrogen bonds. In the crystal, the complex molecules are stacked in columns along the *a* axis.

3D view



Chemical scheme



Structure description

With reference to the title compound, $[Pd(dipic)(bipy)]\cdot H_2O$ (dipic = pyridine-2,6-dicarboxylate; bipy = 2,2′-bipyridine), the crystal structures of related Pd^{II} complexes $[Pd(dipic)(phen)]\cdot 4H_2O$ and $[Pd(dipic23)(bipy)]\cdot 3H_2O$ (phen = 1,10-phenanthroline; dipic23 = pyridine-2,3-dicarboxylate) have been determined previously (Wang & Okabe, 2005).

In the title complex, the central Pd^{II} cation is four-coordinated in a distorted square-planar coordination geometry defined by the N1 and N2 atoms of the bidentate bipy ligand, the O3 and N3 atoms of the di-anionic dipic ligand. An intramolecular C10—H10···O3 hydrogen bond further stabilizes the complex (Fig. 1, Table 1). The tight O—Pd—N and N—Pd—N chelating angles of <O3—Pd1—N3 = 81.07 (10)° and <N1—Pd1—N2 = 80.21 (12)°, and the steric interactions between the non-coordinating carboxylate group and the (N1–C5) pyridyl ring contribute to the distortion of the square plane. The Pd—N and Pd—O bonds are almost equal [1.992 (3)-2.038 (3) Å] and the nearly planar pyridyl rings of the bipy ligand are slightly twisted with a dihedral angle of 12.6 (1)° between them. The dihedral angle between the least-squares plane [maximum deviation = 0.176 (2) Å] of the bipy ligand and the pyridyl ring of the dipic ligand is 30.6 (1)°.

In the crystal structure (Fig. 2), the complex and solvent molecules form intermolecular O—H···O and C—H···O hydrogen bonds (Table 1). The complex molecules

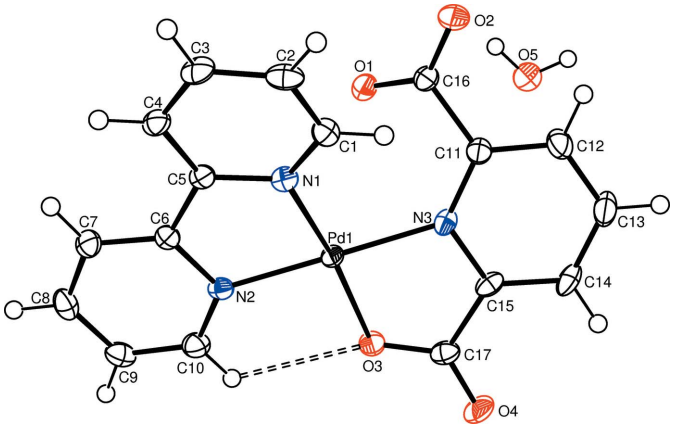


Figure 1
The molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for non-H atoms. The intramolecular hydrogen bond is drawn as a double-dashed line.

are stacked in columns along the *a* axis. In the columns, numerous intermolecular π–π interactions between adjacent pyridyl rings are present. For *Cg*1 (the centroid of ring N1–C5) and *Cg*2^{i} [the centroid of ring N2—C10; symmetry code: (i) x, $\frac{3}{2}-y$, $\frac{1}{2}+z$], the centroid–centroid distance is 3.657 (2) Å and the dihedral angle between the ring planes is 12.4 (2)°.

Synthesis and crystallization

To a solution of $Pd(CH_3CO_2)_2$ (0.2036 g, 0.907 mmol) in acetone (25 ml) and MeOH (5 ml) were added pyridine-2,6-dicarboxylic acid (0.1520 g, 0.910 mmol) and 2,2′-bipyridine (0.1423 g, 0.911 mmol), and stirred for 2 h at room temperature. The precipitate that formed was separated by filtration, washed with acetone, and dried at 333 K, to give a yellow powder (0.3605 g). Yellow crystals suitable for X-ray analysis were obtained by slow evaporation from an ethanol solution at room temperature.

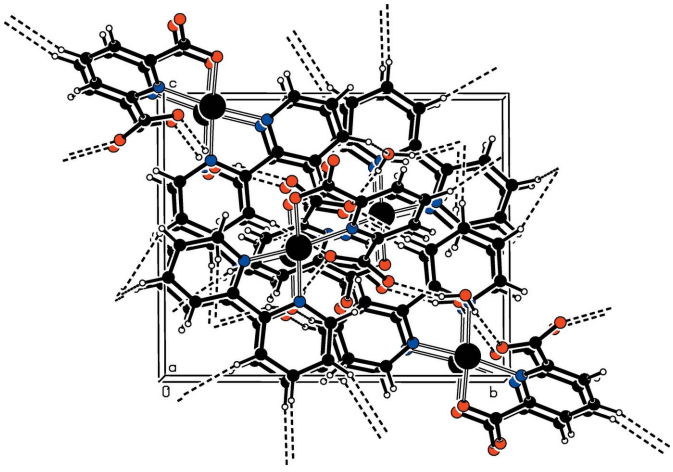


Figure 2
The packing in the crystal structure of the title compound, viewed approximately along the *a* axis. Hydrogen-bonding interactions are drawn as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O1^{i}	0.84	1.96	2.792 (4)	174
O5—H5B···O2^{ii}	0.84	1.99	2.790 (4)	160
C2—H2···O5^{iii}	0.94	2.59	3.460 (5)	154
C3—H3···O2^{iv}	0.94	2.31	3.245 (4)	173
C4—H4···O1^{v}	0.94	2.35	3.261 (4)	162
C8—H8···O5^{v}	0.94	2.47	2.997 (5)	116
C10—H10···O3	0.94	2.55	3.083 (4)	117
C13—H13···O4^{vi}	0.94	2.43	3.336 (5)	161

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x, y, z+1$; (iv) $-x+1, -y+1, -z+2$; (v) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (vi) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$
M_r	445.70
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	12.9031 (10), 12.1751 (10), 10.4256 (7)
β (°)	106.246 (2)
V (Å^3)	1572.4 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.22
Crystal size (mm)	0.17 × 0.11 × 0.06
Data collection	
Diffractometer	PHOTON 100 CMOS detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.683, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	40118, 3110, 2325
R_{int}	0.110
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.061, 1.06
No. of reflections	3110
No. of parameters	235
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.69, −0.71

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x191625 [https://doi.org/10.1107/S2414314619016250]

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Crystal data

$[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$
M_r = 445.70
Monoclinic, $P2_1/c$
a = 12.9031 (10) Å
b = 12.1751 (10) Å
c = 10.4256 (7) Å
β = 106.246 (2)°
V = 1572.4 (2) Å^3
Z = 4
$F(000)$ = 888
D_x = 1.883 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8336 reflections
θ = 2.4–26.0°
μ = 1.22 mm^{-1}
T = 223 K
Rod, yellow
0.17 × 0.11 × 0.06 mm

Data collection

PHOTON 100 CMOS detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.683, T_{max} = 0.745
40118 measured reflections
3110 independent reflections
2325 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 26.1°, θ_{min} = 2.4°
h = −15→15
k = −15→15
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.061
S = 1.06
3110 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2 + 2.4725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.18480 (2)	0.62619 (2)	0.56502 (2)	0.01608 (8)
O1	0.40895 (19)	0.5298 (2)	0.5905 (2)	0.0247 (6)
O2	0.4447 (2)	0.3619 (2)	0.6786 (2)	0.0345 (7)
O3	0.06841 (19)	0.6372 (2)	0.3919 (2)	0.0229 (6)
O4	−0.0568 (2)	0.5284 (2)	0.2619 (2)	0.0313 (7)
N1	0.2794 (2)	0.6223 (3)	0.7542 (2)	0.0179 (6)
N2	0.1816 (2)	0.7845 (2)	0.6120 (3)	0.0172 (6)
N3	0.1930 (2)	0.4707 (2)	0.4962 (2)	0.0169 (6)
C1	0.3089 (3)	0.5325 (3)	0.8287 (3)	0.0201 (8)
H1	0.2861	0.4633	0.7914	0.024*
C2	0.3721 (3)	0.5389 (3)	0.9590 (3)	0.0240 (9)
H2	0.3906	0.4748	1.0107	0.029*
C3	0.4080 (3)	0.6398 (3)	1.0131 (3)	0.0239 (8)
H3	0.4541	0.6448	1.1004	0.029*
C4	0.3758 (3)	0.7334 (3)	0.9383 (3)	0.0220 (8)
H4	0.3984	0.8030	0.9744	0.026*
C5	0.3094 (3)	0.7229 (3)	0.8088 (3)	0.0170 (8)
C6	0.2582 (3)	0.8153 (3)	0.7249 (3)	0.0165 (8)
C7	0.2802 (3)	0.9246 (3)	0.7548 (3)	0.0215 (8)
H7	0.3349	0.9451	0.8314	0.026*
C8	0.2205 (3)	1.0037 (3)	0.6703 (3)	0.0247 (8)
H8	0.2335	1.0787	0.6897	0.030*
C9	0.1419 (3)	0.9715 (3)	0.5575 (4)	0.0246 (8)
H9	0.1002	1.0242	0.4996	0.030*
C10	0.1252 (3)	0.8617 (3)	0.5306 (3)	0.0240 (8)
H10	0.0725	0.8400	0.4527	0.029*
C11	0.2729 (3)	0.3955 (3)	0.5297 (3)	0.0195 (8)
C12	0.2544 (3)	0.2891 (3)	0.4812 (3)	0.0291 (9)
H12	0.3095	0.2363	0.5069	0.035*
C13	0.1559 (3)	0.2602 (3)	0.3956 (4)	0.0308 (9)
H13	0.1419	0.1874	0.3660	0.037*
C14	0.0777 (3)	0.3407 (3)	0.3540 (3)	0.0246 (9)
H14	0.0111	0.3241	0.2924	0.029*
C15	0.0991 (3)	0.4453 (3)	0.4042 (3)	0.0187 (8)
C16	0.3866 (3)	0.4333 (3)	0.6088 (3)	0.0194 (8)
C17	0.0287 (3)	0.5420 (3)	0.3484 (3)	0.0215 (8)
O5	0.4222 (2)	0.3608 (3)	0.2280 (3)	0.0690 (11)
H5A	0.4744	0.3891	0.2854	0.104*
H5B	0.4281	0.2921	0.2325	0.104*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01601 (14)	0.01669 (13)	0.01266 (12)	0.00058 (13)	−0.00074 (9)	−0.00092 (12)
O1	0.0225 (14)	0.0201 (14)	0.0276 (13)	−0.0024 (11)	0.0008 (11)	−0.0002 (11)

O2	0.0296 (15)	0.0246 (15)	0.0370 (15)	0.0053 (13)	−0.0113 (12)	0.0063 (13)
O3	0.0223 (13)	0.0220 (14)	0.0182 (12)	0.0034 (12)	−0.0045 (10)	−0.0004 (11)
O4	0.0222 (15)	0.0333 (16)	0.0290 (14)	−0.0037 (12)	−0.0083 (12)	−0.0014 (12)
N1	0.0173 (15)	0.0217 (15)	0.0152 (13)	0.0002 (14)	0.0055 (11)	0.0002 (13)
N2	0.0152 (15)	0.0223 (16)	0.0143 (14)	0.0021 (13)	0.0042 (12)	−0.0014 (12)
N3	0.0203 (17)	0.0166 (16)	0.0118 (14)	−0.0040 (13)	0.0011 (12)	0.0024 (12)
C1	0.021 (2)	0.019 (2)	0.0208 (18)	0.0001 (16)	0.0075 (16)	0.0022 (15)
C2	0.020 (2)	0.035 (2)	0.0174 (18)	0.0067 (18)	0.0061 (15)	0.0068 (16)
C3	0.0214 (19)	0.036 (2)	0.0111 (15)	0.0022 (18)	−0.0005 (14)	−0.0025 (16)
C4	0.018 (2)	0.029 (2)	0.0185 (18)	0.0009 (16)	0.0035 (15)	−0.0071 (16)
C5	0.0150 (18)	0.023 (2)	0.0145 (16)	0.0006 (16)	0.0067 (14)	−0.0040 (14)
C6	0.0160 (19)	0.0203 (19)	0.0155 (17)	0.0001 (15)	0.0083 (14)	−0.0019 (14)
C7	0.022 (2)	0.025 (2)	0.0183 (18)	−0.0005 (16)	0.0067 (15)	−0.0053 (15)
C8	0.030 (2)	0.0188 (19)	0.030 (2)	0.0003 (17)	0.0165 (17)	−0.0036 (16)
C9	0.022 (2)	0.024 (2)	0.028 (2)	0.0058 (17)	0.0067 (16)	0.0059 (16)
C10	0.0209 (19)	0.027 (2)	0.0217 (17)	0.0026 (17)	0.0024 (15)	−0.0017 (17)
C11	0.0224 (19)	0.018 (2)	0.0155 (16)	−0.0002 (15)	0.0013 (14)	0.0025 (14)
C12	0.035 (2)	0.018 (2)	0.027 (2)	0.0040 (18)	−0.0033 (18)	0.0004 (16)
C13	0.038 (2)	0.019 (2)	0.030 (2)	−0.0077 (18)	−0.0003 (18)	−0.0021 (16)
C14	0.027 (2)	0.026 (2)	0.0161 (17)	−0.0120 (16)	−0.0017 (15)	−0.0018 (15)
C15	0.0164 (19)	0.026 (2)	0.0117 (16)	−0.0042 (16)	0.0008 (14)	0.0025 (14)
C16	0.020 (2)	0.022 (2)	0.0138 (17)	0.0006 (16)	0.0008 (15)	−0.0029 (15)
C17	0.017 (2)	0.030 (2)	0.0168 (18)	0.0010 (17)	0.0034 (16)	−0.0009 (16)
O5	0.043 (2)	0.037 (2)	0.099 (3)	0.0097 (16)	−0.0277 (18)	−0.0245 (19)

Geometric parameters (Å, º)

Pd1—N2	1.992 (3)	C4—H4	0.9400
Pd1—O3	2.004 (2)	C5—C6	1.465 (5)
Pd1—N1	2.009 (2)	C6—C7	1.378 (5)
Pd1—N3	2.038 (3)	C7—C8	1.385 (5)
O1—C16	1.238 (4)	C7—H7	0.9400
O2—C16	1.242 (4)	C8—C9	1.378 (5)
O3—C17	1.296 (4)	C8—H8	0.9400
O4—C17	1.225 (4)	C9—C10	1.371 (5)
N1—C1	1.334 (4)	C9—H9	0.9400
N1—C5	1.361 (4)	C10—H10	0.9400
N2—C10	1.337 (4)	C11—C12	1.387 (5)
N2—C6	1.361 (4)	C11—C16	1.538 (5)
N3—C11	1.350 (4)	C12—C13	1.379 (5)
N3—C15	1.354 (4)	C12—H12	0.9400
C1—C2	1.378 (5)	C13—C14	1.386 (5)
C1—H1	0.9400	C13—H13	0.9400
C2—C3	1.376 (5)	C14—C15	1.375 (5)
C2—H2	0.9400	C14—H14	0.9400
C3—C4	1.377 (5)	C15—C17	1.501 (5)
C3—H3	0.9400	O5—H5A	0.8400
C4—C5	1.388 (4)	O5—H5B	0.8400

N2—Pd1—O3	95.44 (10)	C6—C7—C8	119.0 (3)
N2—Pd1—N1	80.21 (12)	C6—C7—H7	120.5
O3—Pd1—N1	169.28 (10)	C8—C7—H7	120.5
N2—Pd1—N3	172.85 (11)	C9—C8—C7	119.4 (3)
O3—Pd1—N3	81.07 (10)	C9—C8—H8	120.3
N1—Pd1—N3	104.28 (11)	C7—C8—H8	120.3
C17—O3—Pd1	112.2 (2)	C10—C9—C8	119.2 (3)
C1—N1—C5	119.5 (3)	C10—C9—H9	120.4
C1—N1—Pd1	125.9 (2)	C8—C9—H9	120.4
C5—N1—Pd1	114.4 (2)	N2—C10—C9	122.0 (3)
C10—N2—C6	119.3 (3)	N2—C10—H10	119.0
C10—N2—Pd1	124.7 (2)	C9—C10—H10	119.0
C6—N2—Pd1	114.8 (2)	N3—C11—C12	119.9 (3)
C11—N3—C15	119.7 (3)	N3—C11—C16	118.7 (3)
C11—N3—Pd1	130.6 (2)	C12—C11—C16	121.0 (3)
C15—N3—Pd1	109.7 (2)	C13—C12—C11	120.5 (4)
N1—C1—C2	121.4 (3)	C13—C12—H12	119.8
N1—C1—H1	119.3	C11—C12—H12	119.8
C2—C1—H1	119.3	C12—C13—C14	118.7 (3)
C3—C2—C1	119.5 (3)	C12—C13—H13	120.6
C3—C2—H2	120.2	C14—C13—H13	120.6
C1—C2—H2	120.2	C15—C14—C13	119.0 (3)
C2—C3—C4	119.6 (3)	C15—C14—H14	120.5
C2—C3—H3	120.2	C13—C14—H14	120.5
C4—C3—H3	120.2	N3—C15—C14	121.7 (3)
C3—C4—C5	118.7 (3)	N3—C15—C17	114.9 (3)
C3—C4—H4	120.6	C14—C15—C17	122.9 (3)
C5—C4—H4	120.6	O1—C16—O2	128.8 (3)
N1—C5—C4	121.0 (3)	O1—C16—C11	115.4 (3)
N1—C5—C6	114.4 (3)	O2—C16—C11	115.7 (3)
C4—C5—C6	124.3 (3)	O4—C17—O3	124.4 (3)
N2—C6—C7	121.1 (3)	O4—C17—C15	120.1 (3)
N2—C6—C5	113.7 (3)	O3—C17—C15	115.4 (3)
C7—C6—C5	125.2 (3)	H5A—O5—H5B	109.1

C5—N1—C1—C2	−2.0 (5)	C8—C9—C10—N2	1.2 (5)
Pd1—N1—C1—C2	−178.4 (3)	C15—N3—C11—C12	−7.2 (5)
N1—C1—C2—C3	−1.6 (5)	Pd1—N3—C11—C12	171.6 (3)
C1—C2—C3—C4	3.2 (5)	C15—N3—C11—C16	166.2 (3)
C2—C3—C4—C5	−1.3 (5)	Pd1—N3—C11—C16	−15.0 (4)
C1—N1—C5—C4	4.0 (5)	N3—C11—C12—C13	2.0 (6)
Pd1—N1—C5—C4	−179.3 (3)	C16—C11—C12—C13	−171.2 (3)
C1—N1—C5—C6	−170.6 (3)	C11—C12—C13—C14	3.1 (6)
Pd1—N1—C5—C6	6.1 (4)	C12—C13—C14—C15	−3.0 (6)
C3—C4—C5—N1	−2.4 (5)	C11—N3—C15—C14	7.3 (5)
C3—C4—C5—C6	171.7 (3)	Pd1—N3—C15—C14	−171.6 (3)
C10—N2—C6—C7	−1.6 (5)	C11—N3—C15—C17	−164.5 (3)

Pd1—N2—C6—C7	166.6 (3)	Pd1—N3—C15—C17	16.5 (3)
C10—N2—C6—C5	176.6 (3)	C13—C14—C15—N3	−2.2 (5)
Pd1—N2—C6—C5	−15.2 (4)	C13—C14—C15—C17	169.0 (3)
N1—C5—C6—N2	5.9 (4)	N3—C11—C16—O1	−28.4 (4)
C4—C5—C6—N2	−168.6 (3)	C12—C11—C16—O1	144.9 (3)
N1—C5—C6—C7	−176.0 (3)	N3—C11—C16—O2	154.0 (3)
C4—C5—C6—C7	9.6 (6)	C12—C11—C16—O2	−32.6 (5)
N2—C6—C7—C8	2.2 (5)	Pd1—O3—C17—O4	163.9 (3)
C5—C6—C7—C8	−175.8 (3)	Pd1—O3—C17—C15	−20.6 (4)
C6—C7—C8—C9	−1.0 (5)	N3—C15—C17—O4	178.1 (3)
C7—C8—C9—C10	−0.6 (5)	C14—C15—C17—O4	6.3 (5)
C6—N2—C10—C9	−0.1 (5)	N3—C15—C17—O3	2.4 (4)
Pd1—N2—C10—C9	−167.0 (3)	C14—C15—C17—O3	−169.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O1^{i}	0.84	1.96	2.792 (4)	174
O5—H5*B*···O2^{ii}	0.84	1.99	2.790 (4)	160
C2—H2···O5^{iii}	0.94	2.59	3.460 (5)	154
C3—H3···O2^{iv}	0.94	2.31	3.245 (4)	173
C4—H4···O1^{v}	0.94	2.35	3.261 (4)	162
C8—H8···O5^{v}	0.94	2.47	2.997 (5)	116
C10—H10···O3	0.94	2.55	3.083 (4)	117
C13—H13···O4^{vi}	0.94	2.43	3.336 (5)	161

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+1/2, *z*−1/2; (iii) *x*, *y*, *z*+1; (iv) −*x*+1, −*y*+1, −*z*+2; (v) *x*, −*y*+3/2, *z*+1/2; (vi) −*x*, *y*−1/2, −*z*+1/2.