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Poly[[[μ_4-4,4′-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)dipalladium(II)] dihydrate]

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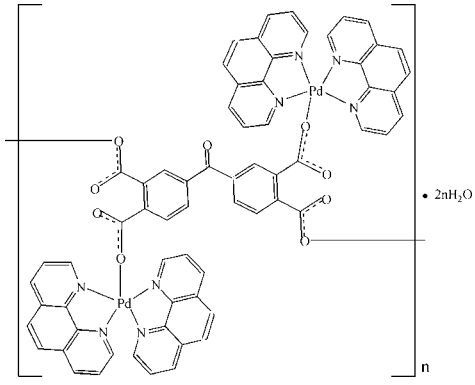
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.114; data-to-parameter ratio = 12.5.

The title compound, $\{[Pd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O\}_n$, was prepared by hydrothermal synthesis and is isostructural with its Cd^{2+}-containing analogue. A twofold rotation axis passes through the carbonyl group of the benzophenone unit. In the asymmetric unit, the Pd atom exhibts a distorted octahedral geometry, consisting of two carboxylate O atoms from two 4,4′-carbonylbis(benzene-3,4-dicarboxylate) anions and four N atoms from two 1,10-phenanthroline ligands. The Pd—N and Pd—O bond lengths are in the ranges 2.391 (3)–2.520 (3) and 2.270 (2)–2.523 (3) Å, respectively. Two neighboring Pd atoms are bridged by 4,4′-carbonylbis(benzene-3,4-dicarboxylate) anions, forming a dinuclear complex, which is further bridged by 4,4′-carbonylbis(benzene-3,4-dicarboxylate) anions to form an infinite chain. Hydrogen bonds link the chains into a three-dimensional structure.

Related literature

For the isostructural Cd^{2+} analogue, see: Gao *et al.* (2007).



Experimental

Crystal data

$[Pd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O$
M_r = 1323.91
Monoclinic, $C2/c$
a = 24.483 (2) Å
b = 10.0027 (10) Å
c = 23.7133 (15) Å
β = 110.786 (2)°
V = 5429.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.74 mm^{-1}
T = 273 (2) K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.917, T_{max} = 0.943
21160 measured reflections
4924 independent reflections
3659 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
S = 1.00
4924 reflections
395 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H2*W*···O1	0.81 (3)	2.18 (4)	2.964 (5)	163 (4)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

he authors thank Shandong University of Technology for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2033).

References

Bruker (2001). *SADABS*, *SAINT-Plus* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, Y.-X., Wang, L.-B. & Niu, Y.-L. (2007). *Acta Cryst.* E**63**, m1844.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, m2312 [**doi:10.1107/S1600536807039050**]

Poly[[[μ_4-4,4'-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-phenanthroline)dipalladium(II)] dihydrate]

Z.-F. Li, S.-W. Wang, Q. Zhang and X.-J. Yu

Comment

As shown on Fig. 1, the palladium cation is hexa-coordinated by two carboxylate oxygen atoms from two 3,3',4,4'-benzophenone tetracarboxylate and four nitrogen atoms from two 1,10-phenanthroline ligand, exhibiting a distorted octahedral geometry. Each two Pd atoms form one circle *via* four carboxylate group belonging two of 3,3',4,4'-benzophenone tetracarboxylate, which are further linked to form one dimensional chain (Fig.2). Interestinfly, the benzophenone carbonyl group (C33═O5) lies on a twofold rotation axis. Moreover, the hydrogen bonds link the chains into a three-dimensional structure (Fig. 3).

Experimental

A mixture of palladium acetate (0.1 mmol), 3,3',4,4'-benzophenone tetracarboxylic acid (0.1 mmol), and 1,10-phenanthroline (0.2 mmol) in 16 ml 1:1 solution of methanol and acetonitrile was sealed in an 25 ml teflon-lined stainless autoclave, and kept at 393 K for 2 days. Colorless, block-shaped crystals were obtained after slowly cooling to room temperature with a yield of 8%. Anal. Calc. for $C_{65}H_{42}N_8O_{11}Pd_2$: C 58.92, H 3.17, N 8.46%; Found: C 58.91, H 3.12, N 8.38%.

Refinement

All H atoms on C atoms were generated geometrically and refined as riding atoms with C–H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of d(H–H) = 1.38 (2) Å, d(O–H) = 0.82 (2) Å, and with a fixed U_{iso} of 0.80 Å^2.

The structure contains solvent accessible voids along *y* axis with the nearest distance of 2.915 Å between O3 and its symmetric site. The position (1/2, 0.766, 3/4) of $\Delta\rho_{max}$ peack (1.46 e A^{-3}) is 0.819 Å to Pd1 atom.

Figures

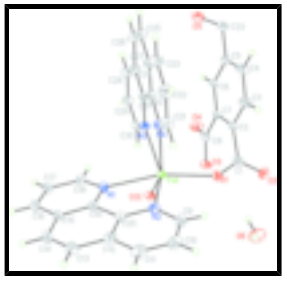

Fig. 1. The coordination of the Pd atom in the title structure, drawn with 30% probability displacement ellipsoids. Atom O3_I has the symmetry positions: (−*x* + 1, *y*, −*z* − 1/2).

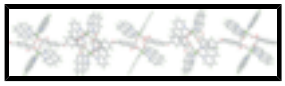

Fig. 2. A view of the chain structure of the title compound.

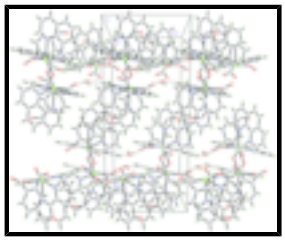

Fig. 3. A view of the packing structure of the title compound.

Poly[[[μ$_4$-4,4'-carbonylbis(benzene-3,4-dicarboxylato)]tetrakis(1,10-\ phenanthroline)dipalladium(II)] dihydrate]

Crystal data

$[Pd_2(C_{17}H_6O_9)(C_{12}H_8N_2)_4]\cdot 2H_2O$	F_{000} = 2672
M_r = 1323.91	D_x = 1.620 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4924 reflections
a = 24.483 (2) Å	θ = 1.8–25.5º
b = 10.0027 (10) Å	μ = 0.74 mm^{-1}
c = 23.7133 (15) Å	*T* = 273 (2) K
β = 110.786 (2)º	Block, colourless
V = 5429.4 (8) Å^3	0.12 × 0.10 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	4924 independent reflections
Radiation source: fine-focus sealed tube	3659 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 273(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −29→29
T_{min} = 0.917, T_{max} = 0.943	*k* = −12→12
21160 measured reflections	*l* = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.114	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 2.9034P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4924 reflections	$\Delta\rho_{max} = 1.46$ e Å^{-3}
395 parameters	$\Delta\rho_{min} = -1.86$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\sigma(F^2)$ 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^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.66566 (15)	0.4950 (4)	−0.05461 (18)	0.0373 (10)
C2	0.62534 (14)	0.4085 (4)	−0.10507 (17)	0.0343 (9)
C3	0.56800 (16)	0.4503 (5)	−0.1303 (2)	0.0555 (13)
H3	0.5561	0.5266	−0.1154	0.067*
C4	0.52765 (16)	0.3801 (5)	−0.1776 (2)	0.0590 (14)
H4	0.4894	0.4110	−0.1942	0.071*
C5	0.54343 (16)	0.2665 (5)	−0.1999 (2)	0.0430 (11)
C6	0.60110 (15)	0.2225 (4)	−0.17500 (19)	0.0370 (10)
H6	0.6122	0.1447	−0.1895	0.044*
C7	0.64201 (14)	0.2932 (4)	−0.12896 (17)	0.0319 (9)
C8	0.70470 (15)	0.2476 (4)	−0.10605 (19)	0.0357 (9)
C9	0.64853 (17)	0.5203 (5)	0.1397 (2)	0.0490 (11)
H9	0.6487	0.5760	0.1083	0.059*
C10	0.63881 (19)	0.5773 (5)	0.1897 (2)	0.0594 (13)
H10	0.6315	0.6684	0.1903	0.071*
C11	0.64011 (19)	0.4991 (5)	0.2371 (2)	0.0594 (13)
H11	0.6336	0.5366	0.2701	0.071*
C12	0.65129 (16)	0.3610 (5)	0.2361 (2)	0.0454 (11)
C13	0.6573 (2)	0.2742 (5)	0.2862 (2)	0.0566 (13)
H13	0.6514	0.3077	0.3202	0.068*
C14	0.67135 (19)	0.1438 (5)	0.2842 (2)	0.0544 (12)
H14	0.6751	0.0888	0.3170	0.065*
C15	0.68055 (15)	0.0892 (5)	0.23266 (18)	0.0420 (10)
C16	0.69707 (16)	−0.0448 (5)	0.2297 (2)	0.0486 (11)
H16	0.7015	−0.1029	0.2617	0.058*

C17	0.70654 (16)	−0.0889 (5)	0.1790 (2)	0.0474 (11)
H17	0.7178	−0.1768	0.1765	0.057*
C18	0.69913 (15)	−0.0010 (4)	0.1317 (2)	0.0423 (10)
H18	0.7058	−0.0327	0.0978	0.051*
C19	0.67424 (14)	0.1712 (4)	0.18226 (18)	0.0355 (9)
C20	0.65990 (14)	0.3125 (4)	0.18437 (18)	0.0364 (9)
C21	0.52649 (17)	0.3400 (5)	0.0298 (2)	0.0550 (13)
H21	0.5424	0.4064	0.0585	0.066*
C22	0.46590 (18)	0.3256 (5)	0.0063 (2)	0.0597 (14)
H22	0.4419	0.3809	0.0189	0.072*
C23	0.44262 (17)	0.2268 (5)	−0.0361 (2)	0.0554 (14)
H23	0.4024	0.2149	−0.0524	0.066*
C24	0.47889 (15)	0.1454 (5)	−0.0545 (2)	0.0463 (11)
C25	0.45739 (17)	0.0411 (5)	−0.0985 (2)	0.0611 (14)
H25	0.4173	0.0278	−0.1160	0.073*
C26	0.49285 (18)	−0.0363 (5)	−0.1150 (2)	0.0596 (14)
H26	0.4772	−0.1010	−0.1445	0.072*
C27	0.55525 (16)	−0.0220 (5)	−0.08808 (19)	0.0433 (10)
C28	0.59378 (18)	−0.1059 (5)	−0.1020 (2)	0.0538 (13)
H28	0.5797	−0.1740	−0.1301	0.065*
C29	0.65242 (17)	−0.0878 (5)	−0.07395 (19)	0.0456 (11)
H29	0.6790	−0.1445	−0.0817	0.055*
C30	0.67154 (15)	0.0188 (4)	−0.03310 (18)	0.0392 (10)
H30	0.7116	0.0321	−0.0150	0.047*
C31	0.57785 (14)	0.0811 (4)	−0.04579 (17)	0.0338 (9)
C32	0.53967 (14)	0.1670 (4)	−0.02838 (18)	0.0366 (9)
C33	0.5000	0.1896 (8)	−0.2500	0.0489 (17)
N1	0.68306 (12)	0.1255 (3)	0.13182 (15)	0.0355 (8)
N2	0.65744 (12)	0.3913 (3)	0.13563 (16)	0.0384 (8)
N3	0.63681 (11)	0.1008 (3)	−0.01866 (14)	0.0348 (8)
N4	0.56281 (13)	0.2633 (4)	0.01335 (18)	0.0434 (9)
O1	0.66798 (11)	0.4721 (3)	−0.00036 (12)	0.0419 (7)
O2	0.68966 (13)	0.5899 (3)	−0.06934 (14)	0.0556 (8)
O3	0.73884 (10)	0.3048 (3)	−0.06008 (12)	0.0411 (7)
O4	0.71905 (11)	0.1556 (3)	−0.13319 (15)	0.0578 (9)
O5	0.5000	0.0672 (6)	−0.2500	0.0717 (16)
O6	0.71087 (16)	0.7293 (4)	0.0615 (2)	0.0735 (11)
Pd1	0.672614 (10)	0.28061 (3)	0.051225 (12)	0.02952 (12)
H2W	0.705 (2)	0.661 (3)	0.042 (2)	0.080*
H1W	0.689 (2)	0.746 (5)	0.080 (2)	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0348 (18)	0.039 (2)	0.035 (2)	0.0049 (17)	0.0085 (15)	0.000 (2)
C2	0.0313 (17)	0.041 (2)	0.027 (2)	0.0024 (16)	0.0061 (14)	0.0044 (19)
C3	0.041 (2)	0.065 (3)	0.051 (3)	0.015 (2)	0.0039 (18)	−0.009 (3)
C4	0.0332 (19)	0.076 (4)	0.054 (3)	0.016 (2)	−0.0017 (18)	−0.009 (3)

C5	0.0329 (18)	0.052 (3)	0.036 (3)	0.0034 (18)	0.0027 (16)	−0.001 (2)
C6	0.0360 (18)	0.040 (3)	0.028 (2)	0.0013 (17)	0.0027 (15)	0.0019 (19)
C7	0.0287 (16)	0.038 (2)	0.026 (2)	−0.0003 (15)	0.0066 (14)	0.0017 (18)
C8	0.0313 (18)	0.044 (3)	0.030 (2)	0.0019 (16)	0.0093 (15)	0.004 (2)
C9	0.051 (2)	0.037 (3)	0.060 (3)	0.006 (2)	0.020 (2)	0.006 (2)
C10	0.065 (3)	0.041 (3)	0.074 (4)	0.005 (2)	0.028 (3)	−0.010 (3)
C11	0.062 (3)	0.059 (3)	0.064 (3)	0.000 (2)	0.031 (2)	−0.023 (3)
C12	0.044 (2)	0.053 (3)	0.043 (3)	−0.005 (2)	0.0210 (17)	−0.012 (2)
C13	0.071 (3)	0.070 (4)	0.038 (3)	−0.012 (3)	0.030 (2)	−0.010 (3)
C14	0.071 (3)	0.056 (3)	0.040 (3)	−0.004 (2)	0.025 (2)	0.009 (3)
C15	0.0382 (19)	0.052 (3)	0.034 (2)	−0.0040 (19)	0.0118 (16)	0.003 (2)
C16	0.045 (2)	0.051 (3)	0.049 (3)	0.003 (2)	0.0149 (19)	0.014 (2)
C17	0.045 (2)	0.041 (3)	0.056 (3)	0.0047 (19)	0.0173 (19)	0.004 (2)
C18	0.0406 (19)	0.038 (3)	0.051 (3)	0.0024 (18)	0.0193 (17)	0.001 (2)
C19	0.0276 (16)	0.046 (3)	0.032 (2)	−0.0023 (16)	0.0108 (14)	0.001 (2)
C20	0.0310 (17)	0.046 (3)	0.034 (2)	−0.0003 (16)	0.0139 (15)	−0.004 (2)
C21	0.046 (2)	0.056 (3)	0.061 (3)	0.006 (2)	0.017 (2)	−0.010 (3)
C22	0.043 (2)	0.063 (3)	0.076 (4)	0.017 (2)	0.025 (2)	0.004 (3)
C23	0.0311 (19)	0.065 (3)	0.068 (4)	0.004 (2)	0.015 (2)	0.004 (3)
C24	0.0306 (18)	0.055 (3)	0.051 (3)	0.0002 (19)	0.0113 (17)	0.006 (2)
C25	0.0303 (19)	0.074 (4)	0.071 (3)	−0.012 (2)	0.008 (2)	−0.009 (3)
C26	0.043 (2)	0.068 (4)	0.061 (3)	−0.018 (2)	0.011 (2)	−0.023 (3)
C27	0.042 (2)	0.050 (3)	0.039 (2)	−0.0088 (19)	0.0148 (17)	−0.004 (2)
C28	0.051 (2)	0.063 (3)	0.046 (3)	−0.006 (2)	0.0155 (19)	−0.017 (3)
C29	0.047 (2)	0.050 (3)	0.042 (3)	0.003 (2)	0.0180 (18)	−0.007 (2)
C30	0.0332 (17)	0.048 (3)	0.036 (2)	0.0047 (17)	0.0121 (15)	0.000 (2)
C31	0.0310 (17)	0.039 (2)	0.029 (2)	−0.0028 (16)	0.0084 (14)	0.0035 (19)
C32	0.0293 (17)	0.042 (2)	0.037 (2)	−0.0041 (17)	0.0104 (15)	0.005 (2)
C33	0.033 (3)	0.058 (5)	0.045 (4)	0.000	0.002 (2)	0.000
N1	0.0354 (15)	0.039 (2)	0.0353 (19)	0.0023 (14)	0.0164 (13)	0.0034 (16)
N2	0.0363 (15)	0.037 (2)	0.043 (2)	0.0006 (14)	0.0147 (13)	0.0009 (18)
N3	0.0266 (13)	0.042 (2)	0.0331 (18)	−0.0027 (13)	0.0077 (12)	−0.0015 (16)
N4	0.0342 (16)	0.048 (2)	0.049 (2)	0.0040 (15)	0.0161 (15)	−0.0023 (19)
O1	0.0530 (15)	0.0407 (18)	0.0297 (16)	0.0017 (13)	0.0119 (11)	−0.0015 (14)
O2	0.0666 (18)	0.0462 (19)	0.053 (2)	−0.0146 (16)	0.0201 (15)	0.0032 (17)
O3	0.0272 (12)	0.059 (2)	0.0339 (16)	−0.0001 (12)	0.0073 (10)	−0.0051 (14)
O4	0.0384 (14)	0.064 (2)	0.068 (2)	0.0075 (15)	0.0145 (14)	−0.021 (2)
O5	0.058 (3)	0.066 (4)	0.067 (4)	0.000	−0.006 (2)	0.000
O6	0.076 (2)	0.074 (3)	0.079 (3)	−0.004 (2)	0.039 (2)	−0.033 (2)
Pd1	0.02651 (15)	0.0337 (2)	0.02745 (19)	0.00278 (11)	0.00847 (10)	0.00078 (13)

Geometric parameters (Å, °)

C1—O2	1.230 (5)	C19—C20	1.461 (6)
C1—O1	1.288 (5)	C20—N2	1.383 (5)
C1—C2	1.522 (5)	C21—N4	1.334 (6)
C2—C3	1.381 (5)	C21—C22	1.395 (6)
C2—C7	1.407 (5)	C21—H21	0.9300
C3—C4	1.393 (6)	C22—C23	1.381 (7)

C3—H3	0.9300	C22—H22	0.9300
C4—C5	1.366 (6)	C23—C24	1.384 (6)
C4—H4	0.9300	C23—H23	0.9300
C5—C6	1.394 (5)	C24—C32	1.411 (5)
C5—C33	1.496 (5)	C24—C25	1.437 (7)
C6—C7	1.386 (5)	C25—C26	1.322 (7)
C6—H6	0.9300	C25—H25	0.9300
C7—C8	1.506 (5)	C26—C27	1.439 (5)
C8—O4	1.243 (5)	C26—H26	0.9300
C8—O3	1.252 (5)	C27—C28	1.387 (6)
C9—N2	1.318 (5)	C27—C31	1.408 (6)
C9—C10	1.410 (7)	C28—C29	1.363 (6)
C9—H9	0.9300	C28—H28	0.9300
C10—C11	1.361 (7)	C29—C30	1.404 (6)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.410 (7)	C30—N3	1.312 (5)
C11—H11	0.9300	C30—H30	0.9300
C12—C20	1.404 (6)	C31—N3	1.370 (4)
C12—C13	1.436 (7)	C31—C32	1.434 (6)
C13—C14	1.354 (7)	C32—N4	1.353 (6)
C13—H13	0.9300	C33—O5	1.224 (8)
C14—C15	1.428 (6)	C33—C5^{i}	1.496 (5)
C14—H14	0.9300	N1—Pd1	2.404 (3)
C15—C16	1.409 (6)	N2—Pd1	2.428 (4)
C15—C19	1.412 (6)	N3—Pd1	2.391 (3)
C16—C17	1.375 (6)	N4—Pd1	2.520 (3)
C16—H16	0.9300	O1—Pd1	2.253 (3)
C17—C18	1.386 (6)	O3—Pd1^{ii}	2.270 (2)
C17—H17	0.9300	O6—H2W	0.81 (3)
C18—N1	1.326 (5)	O6—H1W	0.82 (5)
C18—H18	0.9300	Pd1—O3^{ii}	2.270 (2)
C19—N1	1.367 (5)		
O2—C1—O1	124.4 (4)	C21—C22—H22	121.0
O2—C1—C2	117.2 (4)	C22—C23—C24	120.3 (4)
O1—C1—C2	118.0 (4)	C22—C23—H23	119.8
C3—C2—C7	118.0 (4)	C24—C23—H23	119.8
C3—C2—C1	116.4 (4)	C23—C24—C32	117.8 (4)
C7—C2—C1	125.6 (3)	C23—C24—C25	123.0 (4)
C2—C3—C4	121.2 (4)	C32—C24—C25	119.2 (4)
C2—C3—H3	119.4	C26—C25—C24	122.0 (4)
C4—C3—H3	119.4	C26—C25—H25	119.0
C5—C4—C3	120.9 (4)	C24—C25—H25	119.0
C5—C4—H4	119.5	C25—C26—C27	121.1 (4)
C3—C4—H4	119.5	C25—C26—H26	119.5
C4—C5—C6	118.8 (4)	C27—C26—H26	119.5
C4—C5—C33	121.1 (4)	C28—C27—C31	118.9 (3)
C6—C5—C33	120.1 (4)	C28—C27—C26	122.6 (4)
C7—C6—C5	120.9 (4)	C31—C27—C26	118.4 (4)

C7—C6—H6	119.6	C29—C28—C27	119.5 (4)
C5—C6—H6	119.6	C29—C28—H28	120.3
C6—C7—C2	120.2 (3)	C27—C28—H28	120.3
C6—C7—C8	119.2 (4)	C28—C29—C30	118.2 (4)
C2—C7—C8	120.5 (3)	C28—C29—H29	120.9
O4—C8—O3	124.4 (3)	C30—C29—H29	120.9
O4—C8—C7	118.5 (3)	N3—C30—C29	124.5 (3)
O3—C8—C7	117.1 (4)	N3—C30—H30	117.7
N2—C9—C10	122.6 (5)	C29—C30—H30	117.7
N2—C9—H9	118.7	N3—C31—C27	121.5 (4)
C10—C9—H9	118.7	N3—C31—C32	117.7 (3)
C11—C10—C9	120.1 (5)	C27—C31—C32	120.8 (3)
C11—C10—H10	120.0	N4—C32—C24	122.2 (4)
C9—C10—H10	120.0	N4—C32—C31	119.4 (3)
C10—C11—C12	119.8 (5)	C24—C32—C31	118.4 (4)
C10—C11—H11	120.1	O5—C33—C5	121.0 (3)
C12—C11—H11	120.1	O5—C33—C5^{i}	121.0 (3)
C20—C12—C11	116.3 (4)	C5—C33—C5^{i}	118.1 (6)
C20—C12—C13	120.7 (4)	C18—N1—C19	117.4 (4)
C11—C12—C13	122.8 (5)	C18—N1—Pd1	124.2 (3)
C14—C13—C12	120.4 (4)	C19—N1—Pd1	118.3 (3)
C14—C13—H13	119.8	C9—N2—C20	117.2 (4)
C12—C13—H13	119.8	C9—N2—Pd1	125.8 (3)
C13—C14—C15	121.2 (4)	C20—N2—Pd1	117.1 (3)
C13—C14—H14	119.4	C30—N3—C31	117.4 (3)
C15—C14—H14	119.4	C30—N3—Pd1	122.6 (2)
C16—C15—C19	117.3 (4)	C31—N3—Pd1	120.0 (3)
C16—C15—C14	122.8 (4)	C21—N4—C32	118.3 (3)
C19—C15—C14	119.9 (4)	C21—N4—Pd1	126.4 (3)
C17—C16—C15	119.2 (4)	C32—N4—Pd1	115.2 (3)
C17—C16—H16	120.4	C1—O1—Pd1	132.1 (3)
C15—C16—H16	120.4	C8—O3—Pd1^{ii}	103.2 (2)
C16—C17—C18	119.4 (4)	H2W—O6—H1W	117 (3)
C16—C17—H17	120.3	O1—Pd1—O3^{ii}	103.45 (10)
C18—C17—H17	120.3	O1—Pd1—N3	109.11 (11)
N1—C18—C17	123.8 (4)	O3^{ii}—Pd1—N3	83.34 (10)
N1—C18—H18	118.1	O1—Pd1—N1	161.94 (11)
C17—C18—H18	118.1	O3^{ii}—Pd1—N1	81.65 (10)
N1—C19—C15	122.8 (4)	N3—Pd1—N1	88.57 (12)
N1—C19—C20	117.9 (4)	O1—Pd1—N2	93.84 (11)
C15—C19—C20	119.2 (4)	O3^{ii}—Pd1—N2	121.06 (10)
N2—C20—C12	123.9 (4)	N3—Pd1—N2	142.04 (11)
N2—C20—C19	117.5 (4)	N1—Pd1—N2	69.10 (12)
C12—C20—C19	118.5 (4)	O1—Pd1—N4	91.32 (11)
N4—C21—C22	123.3 (5)	O3^{ii}—Pd1—N4	150.49 (11)
N4—C21—H21	118.4	N3—Pd1—N4	67.60 (11)
C22—C21—H21	118.4	N1—Pd1—N4	92.18 (11)

C23—C22—C21	118.1 (5)	N2—Pd1—N4	82.48 (11)
C23—C22—H22	121.0		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H2W···O1	0.81 (3)	2.18 (4)	2.964 (5)	163 (4)

Fig. 1

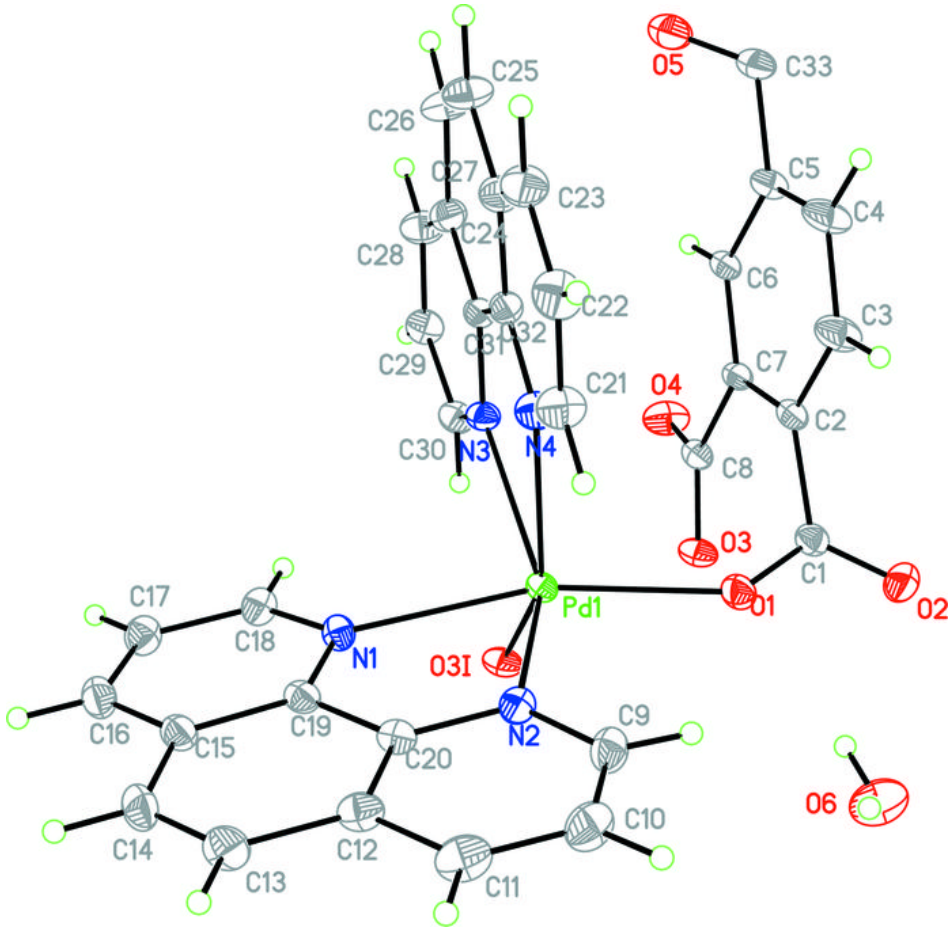
O5
C33
C25
C26
C27
C23
C5
C4
C24
C28
C6
C22
C3
C29
C31
C32
C7
C21
O4
C30
N3
N4
C2
C8
O3
C1
C17
Pd1
O1
O2
C18
N1
O3I
C16
C15
C19
N2
C9
C20
O6
C10
C14
C12
C13
C11

Fig. 2

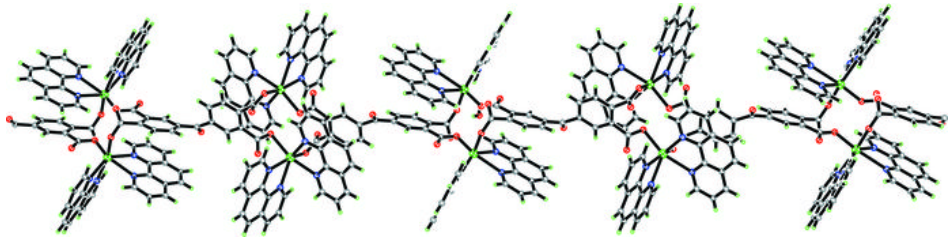

Fig. 3