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Poly[aqua(2,2′-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]

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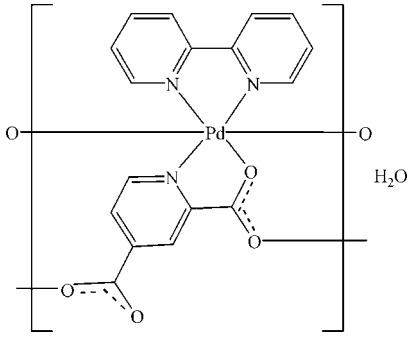
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.046; data-to-parameter ratio = 12.3.

The asymmetric unit of the title compound, $\{[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O\}_n$, contains one palladium cation chelated by one 2,2′-bipyridine ligand and one pyridine-2,4-dicarboxylate ligand, further coordinated by two carboxylate O atoms belonging to two neighbouring independent pyridine-2,4-dicarboxylate ligands. The Pd atom exhibits octahedral geometry involving three N and three O atoms. Each pair of neighbouring Pd^{2+} cations is bridged by two independent pyridine-2,4-dicarboxylate ligands, which are further coordinated to a third Pd^{2+} cation *via* a carboxylate O atom to form corrugated layers parallel to the (101) plane.

Related literature

For related literature, see: An *et al.* (2000); Baroni *et al.* (1996); Go *et al.* (2004); Hundal *et al.* (2002); Li *et al.* (1993)



Experimental

Crystal data

$[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$
M_r = 445.72
Monoclinic, $P2_1/c$
a = 11.8236 (2) Å
b = 14.7796 (5) Å
c = 9.9352 (5) Å
β = 110.987 (1)°
V = 1620.98 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 293 (2) K
0.43 × 0.28 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.631, T_{max} = 0.781
12911 measured reflections
2958 independent reflections
2620 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.046
S = 1.00
2958 reflections
241 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O2^{i}	0.82 (4)	1.95 (2)	2.731 (3)	157 (6)

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2042).

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supplementary materials

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Poly[aqua(2,2'-bipyridine)(μ_3-pyridine-2,4-dicarboxylato)palladium(II)]

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Comment

Complexes containing carboxyl acids have been the interest of chemists these years due to their potential applications, such as catalysis, optics, information storage, medicine, molecular electrochemistry, biochemistry and biological pharmaceutics (Li *et al.* (1993); Go *et al.* (2004)). Thus far, *N*-containing aromatic carboxyl acid has been widely used in dye intermediate, organic synthesis, sensitization material, functional pigment, adipiodone and acetrizoic acid (An *et al.* (2000). Pyridine carboxylic acid is also a good ligand in coordination chemistry due to its strong coordination ability and versatile coordination modes, so much attention has been paid to it in these decades (Baroni *et al.* (1996); Hundal *et al.* (2002)). Herein, we report the new complex - poly[(2,2'-bipyridine)palladium(II)(pyridine-2,4-dicarboxylato)acqua].

The title compound contains one palladium cation chelated by one 2,2'-bipyridine ligand and one pyridine-2,4-dicarboxylate ligand, further coordinated by two carboxylate groups belonging to two neighboring independent pyridine-2,4-dicarboxylate ligands (Fig. 1). Pd atom is hexa-coordinated exhibiting octahedron geometry containing three N and three O atoms. Each two neighboring Pd^{2+}-cations are bridged by two independent pyridine-2,4-dicarboxylate ligands, which are further coordinated to the third Pd^{2+}-cation with carboxylate oxygen atom to form corrugated layers parallel to the (1 0 1) plane (Fig. 2).

Experimental

A mixture of palladium acetate (1 mmol), pyridine-2,4-dicarboxylic acid (1 mmol), and 2,2-bipyridine (2 mmol) in mixed 1:1 solvent of H_2O and ethanol in a 25 ml teflon-lined stainless steel autoclave was kept at 473 K for 10 days. Red crystals were obtained after cooling to room temperature with a yield of 22%. Anal. Calc. for $C_{17}H_{13}N_3O_5Pd$: C 45.77, H 2.47, N 9.42%; Found: 45.71, H 2.52, N 9.40%.

Refinement

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 (1) Å, and refined freely. All other H atoms were placed in calculated positions with a C–H bond distance of 0.93%A and U_{iso}(H) = 1.2U_{eq}(C).

Figures

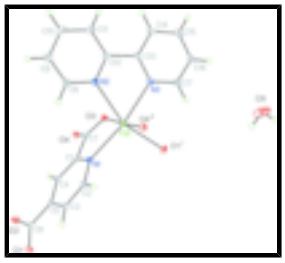

Fig. 1. A view of the title compound with the numbering scheme. Displacement ellipsoids are drawn with 30% probability. H atoms are presented as a spheres of arbitrary radius. Symmetry codes: (i) −*x* + 1, *y* + 1/2, −*z* + 1/2; (ii) *x*, −*y* + 1/2, *z* + 1/2.

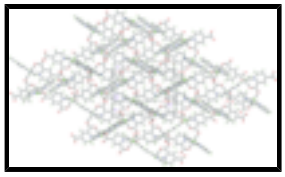

Fig. 2. A view of corrugated layers parallel to the (1 0 1) plane.

Poly[aqua(2,2'-bipyridine)(μ$_3$-pyridine-2,4-dicarboxylato)palladium(II)]

Crystal data

$[Pd(C_7H_3NO_4)(C_{10}H_8N_2)]\cdot H_2O$	F_{000} = 888
M_r = 445.72	D_x = 1.826 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2958 reflections
a = 11.8236 (2) Å	θ = 2.6–25.5º
b = 14.7796 (5) Å	μ = 1.18 mm^{-1}
c = 9.9352 (5) Å	T = 293 (2) K
β = 110.9870 (10)º	Block, red
V = 1620.98 (10) Å^3	0.43 × 0.28 × 0.22 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	2958 independent reflections
Radiation source: fine-focus sealed tube	2620 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 293(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −14→14
T_{min} = 0.631, T_{max} = 0.781	k = −17→17
12911 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.020$

$wR(F^2) = 0.046$

$S = 1.00$

2958 reflections

241 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0184P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.007$

$\Delta\rho_{max} = 0.36$ e Å^{-3}

$\Delta\rho_{min} = -0.61$ e Å^{-3}

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 $F^2 > 2\sigma(F^2)$ 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}
Pd1	0.255492 (13)	0.317737 (9)	0.101199 (14)	0.02804 (6)
C1	0.33154 (16)	0.11459 (12)	0.04854 (18)	0.0294 (4)
C2	0.40267 (19)	0.14676 (14)	0.28598 (19)	0.0374 (5)
H2	0.4112	0.1862	0.3619	0.045*
C3	0.45769 (19)	0.06187 (13)	0.3168 (2)	0.0368 (5)
H3	0.5044	0.0475	0.4116	0.044*
C4	0.38032 (17)	0.02680 (13)	0.07263 (19)	0.0321 (4)
H4	0.3690	−0.0122	−0.0046	0.039*
C5	0.44442 (17)	−0.00109 (12)	0.20991 (19)	0.0318 (4)
C6	0.49924 (19)	−0.09614 (14)	0.2425 (2)	0.0384 (5)
C7	0.27151 (17)	0.15279 (14)	−0.09911 (19)	0.0309 (4)
C8	0.0011 (2)	0.22777 (17)	0.0816 (2)	0.0513 (6)
H8	0.0522	0.1895	0.1512	0.062*
C9	−0.1189 (3)	0.2124 (2)	0.0344 (3)	0.0650 (7)
H9	−0.1508	0.1647	0.0704	0.078*
C10	−0.1918 (3)	0.2688 (2)	−0.0673 (3)	0.0691 (8)
H10	−0.2751	0.2594	−0.1030	0.083*
C11	−0.1428 (2)	0.3405 (2)	−0.1186 (3)	0.0585 (7)
H11	−0.1930	0.3796	−0.1877	0.070*
C12	−0.02156 (19)	0.35290 (15)	−0.06706 (19)	0.0386 (5)

C13	0.03749 (19)	0.42873 (14)	−0.11791 (19)	0.0375 (5)
C14	−0.0261 (2)	0.49206 (17)	−0.2185 (2)	0.0538 (6)
H14	−0.1102	0.4888	−0.2581	0.065*
C15	0.0332 (3)	0.55996 (18)	−0.2608 (3)	0.0673 (8)
H15	−0.0099	0.6024	−0.3290	0.081*
C16	0.1545 (3)	0.56407 (17)	−0.2021 (3)	0.0643 (7)
H16	0.1979	0.6087	−0.2287	0.077*
C17	0.2120 (2)	0.49978 (16)	−0.1013 (2)	0.0502 (6)
H17	0.2959	0.5028	−0.0589	0.060*
N1	0.33959 (16)	0.17305 (10)	0.15486 (16)	0.0329 (4)
N2	0.04991 (17)	0.29603 (12)	0.03223 (17)	0.0394 (4)
N3	0.15557 (16)	0.43315 (11)	−0.06002 (17)	0.0392 (4)
O1	0.57118 (13)	−0.10790 (10)	0.36799 (14)	0.0448 (4)
O2	0.46972 (18)	−0.15543 (11)	0.14916 (18)	0.0658 (5)
O3	0.23331 (13)	0.23406 (10)	−0.11209 (13)	0.0414 (4)
O4	0.26788 (13)	0.10078 (9)	−0.19922 (13)	0.0400 (3)
O5	0.3824 (2)	0.7288 (3)	0.3790 (3)	0.1309 (11)
H1W	0.406 (5)	0.693 (3)	0.447 (4)	0.196*
H2W	0.437 (3)	0.749 (4)	0.354 (5)	0.196*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02882 (10)	0.02435 (9)	0.02583 (9)	0.00097 (6)	0.00355 (7)	0.00026 (5)
C1	0.0268 (10)	0.0330 (10)	0.0274 (9)	−0.0022 (8)	0.0085 (8)	−0.0001 (8)
C2	0.0477 (13)	0.0372 (11)	0.0248 (9)	0.0067 (10)	0.0100 (9)	−0.0001 (8)
C3	0.0425 (12)	0.0403 (12)	0.0263 (9)	0.0072 (9)	0.0107 (9)	0.0061 (8)
C4	0.0321 (10)	0.0341 (10)	0.0292 (9)	−0.0002 (8)	0.0099 (8)	−0.0023 (8)
C5	0.0304 (10)	0.0327 (10)	0.0329 (10)	0.0035 (8)	0.0118 (9)	0.0040 (8)
C6	0.0361 (12)	0.0360 (11)	0.0424 (12)	0.0050 (9)	0.0131 (10)	0.0020 (9)
C7	0.0279 (10)	0.0337 (11)	0.0294 (10)	−0.0060 (8)	0.0081 (8)	0.0001 (8)
C8	0.0525 (15)	0.0548 (15)	0.0444 (12)	−0.0103 (12)	0.0147 (12)	0.0050 (11)
C9	0.0555 (17)	0.0892 (19)	0.0515 (15)	−0.0251 (16)	0.0205 (14)	−0.0021 (14)
C10	0.0431 (15)	0.110 (2)	0.0526 (15)	−0.0217 (16)	0.0156 (13)	−0.0082 (16)
C11	0.0391 (14)	0.092 (2)	0.0397 (12)	0.0044 (13)	0.0090 (11)	0.0014 (12)
C12	0.0368 (12)	0.0492 (12)	0.0284 (10)	0.0046 (10)	0.0099 (9)	−0.0048 (9)
C13	0.0392 (12)	0.0433 (12)	0.0280 (9)	0.0121 (9)	0.0096 (9)	−0.0008 (8)
C14	0.0501 (14)	0.0592 (15)	0.0459 (13)	0.0177 (12)	0.0096 (11)	0.0087 (11)
C15	0.076 (2)	0.0638 (18)	0.0600 (16)	0.0267 (15)	0.0218 (15)	0.0285 (14)
C16	0.072 (2)	0.0581 (16)	0.0673 (16)	0.0076 (14)	0.0310 (15)	0.0253 (13)
C17	0.0493 (14)	0.0469 (14)	0.0575 (13)	0.0045 (11)	0.0230 (12)	0.0138 (11)
N1	0.0384 (10)	0.0313 (9)	0.0277 (8)	0.0023 (7)	0.0103 (8)	0.0012 (6)
N2	0.0373 (10)	0.0458 (10)	0.0324 (9)	−0.0016 (8)	0.0091 (8)	−0.0011 (8)
N3	0.0404 (10)	0.0388 (10)	0.0373 (9)	0.0068 (8)	0.0127 (8)	0.0054 (7)
O1	0.0462 (9)	0.0494 (9)	0.0357 (8)	0.0193 (7)	0.0110 (7)	0.0093 (6)
O2	0.0705 (13)	0.0407 (9)	0.0629 (10)	0.0143 (9)	−0.0043 (9)	−0.0124 (8)
O3	0.0512 (10)	0.0362 (8)	0.0293 (7)	0.0036 (7)	0.0054 (7)	0.0043 (6)
O4	0.0466 (9)	0.0449 (8)	0.0253 (6)	0.0012 (7)	0.0089 (6)	−0.0022 (6)

O5	0.0622 (15)	0.249 (4)	0.0731 (16)	−0.003 (2)	0.0136 (13)	0.0545 (19)

Geometric parameters (Å, °)

Pd1—O1^{i}	2.2476 (14)	C8—H8	0.9300
Pd1—O4^{ii}	2.2793 (13)	C9—C10	1.354 (4)
Pd1—N2	2.2995 (18)	C9—H9	0.9300
Pd1—N1	2.3380 (15)	C10—C11	1.389 (4)
Pd1—N3	2.3485 (16)	C10—H10	0.9300
Pd1—O3	2.3854 (13)	C11—C12	1.351 (3)
C1—N1	1.341 (2)	C11—H11	0.9300
C1—C4	1.405 (3)	C12—N2	1.340 (3)
C1—C7	1.493 (2)	C12—C13	1.501 (3)
C2—N1	1.307 (2)	C13—N3	1.307 (3)
C2—C3	1.396 (3)	C13—C14	1.379 (3)
C2—H2	0.9300	C14—C15	1.374 (4)
C3—C5	1.378 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.342 (4)
C4—C5	1.365 (3)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.371 (3)
C5—C6	1.532 (3)	C16—H16	0.9300
C6—O2	1.232 (2)	C17—N3	1.334 (3)
C6—O1	1.244 (2)	C17—H17	0.9300
C7—O4	1.246 (2)	O1—Pd1^{iii}	2.2476 (14)
C7—O3	1.274 (3)	O4—Pd1^{iv}	2.2793 (13)
C8—N2	1.340 (3)	O5—H1W	0.82 (4)
C8—C9	1.344 (4)	O5—H2W	0.83 (4)
O1^{i}—Pd1—O4^{ii}	81.48 (5)	C8—C9—H9	121.1
O1^{i}—Pd1—N2	157.48 (6)	C10—C9—H9	121.1
O4^{ii}—Pd1—N2	93.71 (5)	C9—C10—C11	120.4 (3)
O1^{i}—Pd1—N1	97.10 (6)	C9—C10—H10	119.8
O4^{ii}—Pd1—N1	113.28 (5)	C11—C10—H10	119.8
N2—Pd1—N1	104.96 (6)	C12—C11—C10	119.3 (2)
O1^{i}—Pd1—N3	87.09 (6)	C12—C11—H11	120.4
O4^{ii}—Pd1—N3	93.98 (5)	C10—C11—H11	120.4
N2—Pd1—N3	71.23 (6)	N2—C12—C11	119.9 (2)
N1—Pd1—N3	152.73 (5)	N2—C12—C13	118.00 (19)
O1^{i}—Pd1—O3	100.33 (5)	C11—C12—C13	122.1 (2)
O4^{ii}—Pd1—O3	177.49 (5)	N3—C13—C14	120.3 (2)
N2—Pd1—O3	83.96 (5)	N3—C13—C12	116.20 (17)
N1—Pd1—O3	68.34 (5)	C14—C13—C12	123.5 (2)
N3—Pd1—O3	84.39 (5)	C15—C14—C13	120.8 (2)
N1—C1—C4	123.47 (16)	C15—C14—H14	119.6
N1—C1—C7	113.89 (16)	C13—C14—H14	119.6
C4—C1—C7	122.56 (16)	C16—C15—C14	118.9 (2)
N1—C2—C3	122.70 (18)	C16—C15—H15	120.5

N1—C2—H2	118.6	C14—C15—H15	120.5
C3—C2—H2	118.6	C15—C16—C17	117.3 (2)
C5—C3—C2	121.52 (17)	C15—C16—H16	121.4
C5—C3—H3	119.2	C17—C16—H16	121.4
C2—C3—H3	119.2	N3—C17—C16	124.4 (2)
C5—C4—C1	119.74 (16)	N3—C17—H17	117.8
C5—C4—H4	120.1	C16—C17—H17	117.8
C1—C4—H4	120.1	C2—N1—C1	116.59 (16)
C4—C5—C3	115.79 (17)	C2—N1—Pd1	122.92 (13)
C4—C5—C6	121.96 (17)	C1—N1—Pd1	120.34 (12)
C3—C5—C6	122.25 (16)	C8—N2—C12	120.1 (2)
O2—C6—O1	124.2 (2)	C8—N2—Pd1	122.97 (15)
O2—C6—C5	120.57 (18)	C12—N2—Pd1	116.90 (14)
O1—C6—C5	115.17 (18)	C13—N3—C17	118.32 (18)
O4—C7—O3	126.28 (16)	C13—N3—Pd1	117.44 (13)
O4—C7—C1	114.81 (17)	C17—N3—Pd1	124.14 (15)
O3—C7—C1	118.86 (16)	C6—O1—Pd1^{iii}	117.87 (13)
N2—C8—C9	122.6 (2)	C7—O3—Pd1	118.48 (10)
N2—C8—H8	118.7	C7—O4—Pd1^{iv}	109.98 (12)
C9—C8—H8	118.7	H1W—O5—H2W	114 (3)
C8—C9—C10	117.8 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O2^{ii}	0.82 (4)	1.95 (2)	2.731 (3)	157 (6)

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

Fig. 1

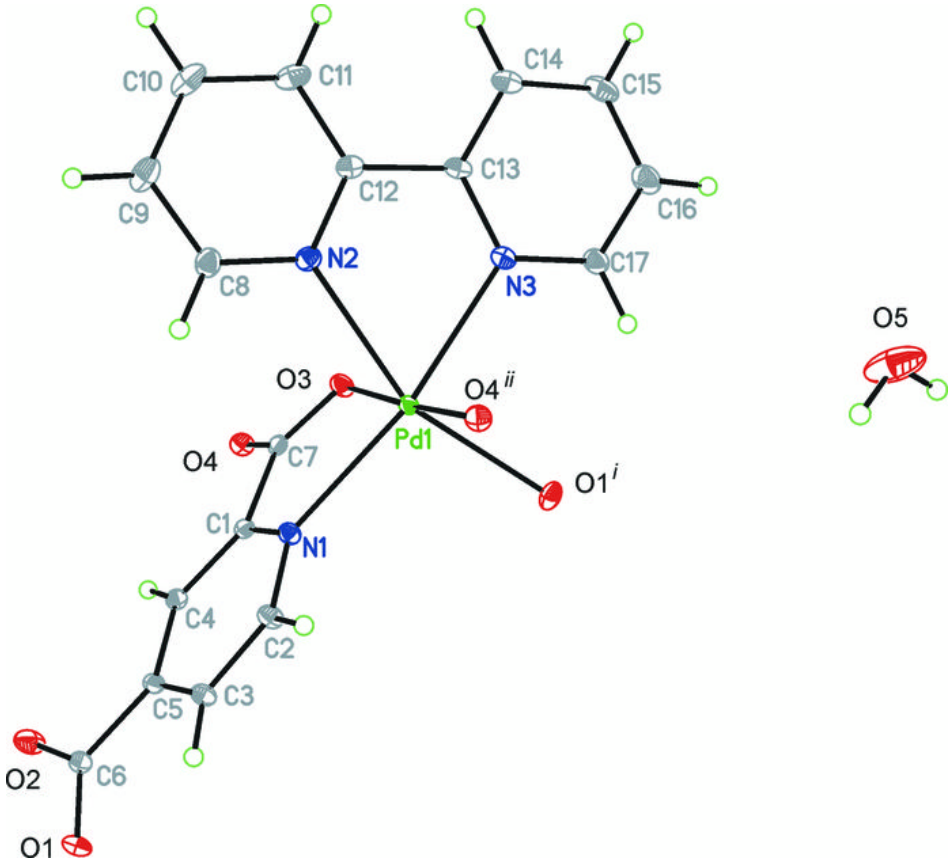
C10
C11
C14
C15
C9
C12
C13
C16
N2
C8
N3
C17
O5
O3
O4 ii
Pd1
O4
C7
O1 i
C1
N1
C4
C2
C5
C3
O2
C6
O1

Fig. 2