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Bis[2,3-bis(pyridin-2-yl)pyrazine-κ^2N^2,N^3]-palladium(II) dinitrate acetonitrile monosolvate

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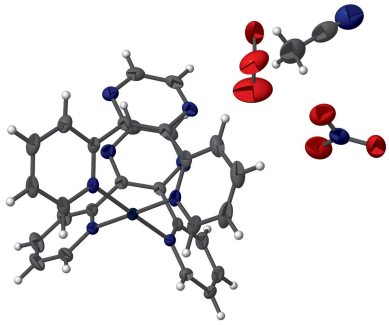
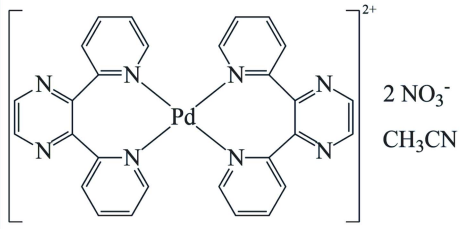
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Pd(C_{14}H_{10}N_4)_2](NO_3)_2\cdot CH_3CN$, consists of a cationic Pd^{II} complex, two anions and one lattice solvent molecule, all in general positions. In the complex, the Pd^{II} cation is four-coordinated in a slightly distorted square-planar geometry defined by the four N atoms of two bidentate 2,3-di-2-pyridylpyrazine ligands. The complex, anions and solvent molecule are linked by weak C—H···O 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, $[Pd(dpp)_2](NO_3)_2\cdot CH_3CN$ (dpp = 2,3-di-2-pyridylpyrazine), the crystal structures of related dpp-Pd^{II} complexes $[PdX_2(dpp)]$ have been determined previously [X = Cl (Ha, 2011*a*,*b*); X = Br (Ha, 2011*c*); X = I (Ha, 2011*d*); X = SCN (Ha, 2012)], and a heterometallic complex has been also reported, namely $[Ru(bipy)_2(\mu_2\text{-dpp})PdCl_2](PF_6)_2$, where bipy is 2,2′-bipyridine (Yam *et al.*, 1994).

The title compound consists of a cationic Pd^{II} complex $[Pd(dpp)_2]^{2+}$, two NO_3^- anions and one solvent CH_3CN molecule (Fig. 1). In the complex, the central Pd^{II} cation is four-coordinated in a slightly distorted square-planar geometry defined by the pyridyl N3, N4, N7 and N8 atoms of the two bidentate dpp ligands. The tight N—Pd—N chelating angles of N3—Pd1—N4 = 86.99 (7)° and N7—Pd1—N8 = 85.98 (7)° contribute to the distortion of the square-plane. The Pd—N bond lengths are almost equal [2.0170 (18) to 2.0286 (19) Å]. In the crystal, the pyridine rings are considerably inclined to the least-squares plane of the $[PdN_4]$ unit [maximum deviation = 0.0204 (7) Å], with dihedral angles of 70.56 (7) (ring N3···C9), 67.63 (6) (ring N4···C14), 71.32 (6) (ring N7···C23) and 71.64 (7)° (ring N8···C28). The nearly planar pyrazine rings [maximum deviation = 0.027 (2) Å] are fairly perpendicular to the $[PdN_4]$ unit plane, with dihedral angles of 82.07 (7) (ring N1···C4) and 84.20 (7)° (ring N5···C18).

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O4^{i}	0.94	2.43	3.344 (3)	164
C4—H4···O1	0.94	2.51	3.330 (4)	146
C9—H9···O2^{ii}	0.94	2.40	3.113 (4)	133
C14—H14···O5^{iii}	0.94	2.43	3.257 (3)	147
C17—H17···O6^{i}	0.94	2.43	3.343 (3)	164
C22—H22···O3^{iv}	0.94	2.45	3.273 (5)	146
C23—H23···O2^{ii}	0.94	2.54	3.275 (4)	136
C29—H29A···O1	0.97	2.58	3.405 (5)	144
C29—H29C···O4	0.97	2.51	3.459 (4)	167

Symmetry codes: (i) $x+1, y, z$; (ii) $x, y+1, z$; (iii) $x+1, y+1, z$; (iv) $-x+1, -y+1, -z$.

In the crystal structure (Fig. 2), the complex, anions and solvent molecules form intermolecular weak C—H···O hydrogen bonds (Table 1). The complex molecules are stacked in columns along the *a* axis. In the columns, numerous intra- and intermolecular π–π interactions between adjacent six-membered rings are present. For *Cg*1 (the centroid of ring N4···C14) and *Cg*1^{i} [symmetry code: (i) $-x+2, -y+2, -z+1$), the centroid-to-centroid separation is 3.688 (2) Å and the planes are parallel and shifted by 1.683 Å.

Synthesis and crystallization

To a solution of 2,3-di-2-pyridylpyrazine (0.303 g, 1.293 mmol) in acetone (30 ml) was added $Pd(NO_3)_2{\cdot}2H_2O$ (0.170 g, 0.637 mmol) and stirred for 1 h at room temperature. The formed precipitate was recrystallized from MeOH/ether, washed with ether, and dried under vacuum, to give a white powder (0.378 g). Crystals suitable for X-ray analysis were obtained by slow evaporation of a MeOH/CH_3CN solution, at room temperature.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pd(C_{14}H_{10}N_4)_2](NO_3)_2{\cdot}C_2H_3N$
M_r	739.99
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	223
a, b, c (Å)	10.2013 (4), 11.6159 (5), 14.2762 (6)
α, β, γ (°)	90.9753 (16), 109.2479 (14), 109.9435 (14)
V (Å^3)	1485.28 (11)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.69
Crystal size (mm)	0.22 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker *APEX2*, PHOTON 100 detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.699, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38859, 5889, 5399
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.066, 1.06
No. of reflections	5889
No. of parameters	434
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.89, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014/7* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

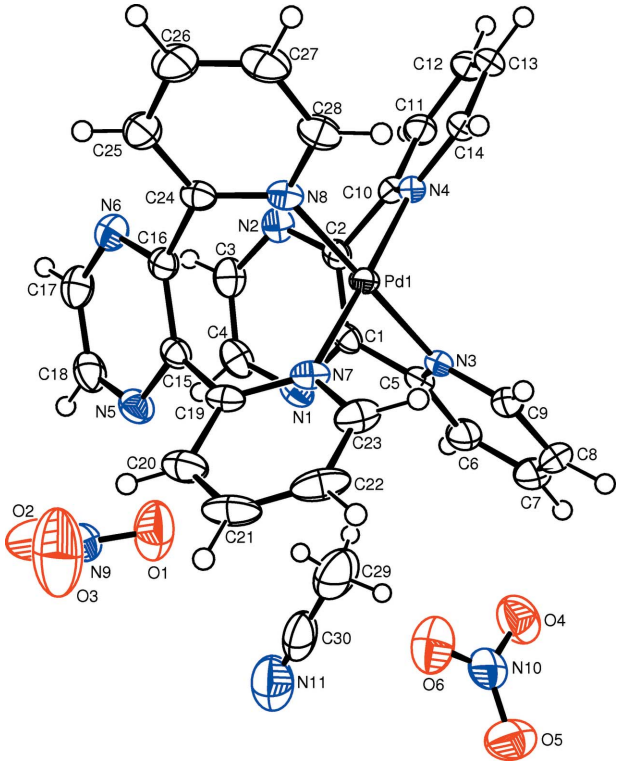


Figure 1
The molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for non-H atoms.

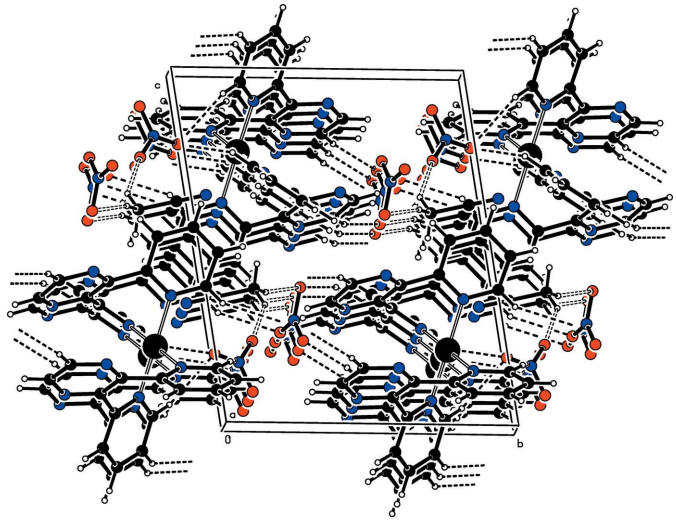


Figure 2
The packing in the crystal structure of the title compound, viewed approximately along the *a* axis. Hydrogen-bonding interactions are drawn as dashed lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The highest peak (0.89 e Å^{-3}) and the deepest hole (−0.49 e Å^{-3}) in the last difference-Fourier map are located 1.02 and 0.97 Å, respectively, from atom O3.

Acknowledgements

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full crystallographic data

IUCrData (2021). **6**, x210153 [https://doi.org/10.1107/S241431462100153X]

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Crystal data

$[Pd(C_{14}H_{10}N_4)_2](NO_3)_2\cdot C_2H_3N$
M_r = 739.99
Triclinic, $P\overline{1}$
a = 10.2013 (4) Å
b = 11.6159 (5) Å
c = 14.2762 (6) Å
α = 90.9753 (16)°
β = 109.2479 (14)°
γ = 109.9435 (14)°
V = 1485.28 (11) Å^3
Z = 2
$F(000)$ = 748
D_x = 1.655 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9802 reflections
θ = 2.3–28.3°
μ = 0.69 mm^{-1}
T = 223 K
Block, colorless
0.22 × 0.15 × 0.09 mm

Data collection

Bruker APEX2, PHOTON 100 detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.699, T_{max} = 0.745
38859 measured reflections
5889 independent reflections
5399 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.1°, θ_{min} = 2.2°
h = −12→12
k = −14→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.066
S = 1.06
5889 reflections
434 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 1.3932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Special details

Refinement. Hydrogen atoms bonded to C atoms were positioned geometrically and allowed to ride on their parent atoms: C—H = 0.94 or 0.97 Å, with isotropic displacements U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.85573 (2)	0.80002 (2)	0.21420 (2)	0.02031 (6)
N1	0.8010 (2)	0.47002 (17)	0.32663 (14)	0.0296 (4)
N2	1.1007 (2)	0.62333 (18)	0.41615 (14)	0.0300 (4)
N3	0.70063 (19)	0.72337 (16)	0.27734 (14)	0.0243 (4)
N4	1.00126 (19)	0.87763 (16)	0.35473 (13)	0.0226 (4)
N5	0.8194 (2)	0.46396 (17)	0.07565 (15)	0.0318 (4)
N6	1.1185 (2)	0.61800 (19)	0.15483 (15)	0.0316 (4)
N7	0.71597 (19)	0.71968 (16)	0.07375 (13)	0.0249 (4)
N8	1.01151 (19)	0.87359 (16)	0.15207 (13)	0.0243 (4)
C1	0.8420 (2)	0.59294 (19)	0.34974 (15)	0.0228 (4)
C2	0.9924 (2)	0.6705 (2)	0.39218 (15)	0.0232 (4)
C3	1.0584 (3)	0.5018 (2)	0.39210 (18)	0.0342 (5)
H3	1.1317	0.4662	0.4075	0.041*
C4	0.9105 (3)	0.4261 (2)	0.34529 (18)	0.0336 (5)
H4	0.8864	0.3415	0.3261	0.040*
C5	0.7133 (2)	0.6331 (2)	0.33404 (16)	0.0259 (5)
C6	0.6064 (3)	0.5744 (2)	0.3748 (2)	0.0380 (6)
H6	0.6146	0.5096	0.4121	0.046*
C7	0.4865 (3)	0.6125 (3)	0.3599 (2)	0.0478 (7)
H7	0.4132	0.5743	0.3874	0.057*
C8	0.4767 (3)	0.7063 (3)	0.3047 (2)	0.0470 (7)
H8	0.3977	0.7344	0.2950	0.056*
C9	0.5843 (2)	0.7592 (2)	0.2632 (2)	0.0350 (6)
H9	0.5757	0.8223	0.2239	0.042*
C10	1.0482 (2)	0.8070 (2)	0.42188 (16)	0.0233 (4)
C11	1.1519 (2)	0.8600 (2)	0.51676 (17)	0.0308 (5)
H11	1.1821	0.8097	0.5635	0.037*
C12	1.2106 (3)	0.9870 (2)	0.54251 (19)	0.0364 (6)
H12	1.2824	1.0240	0.6064	0.044*
C13	1.1629 (3)	1.0586 (2)	0.47366 (19)	0.0342 (5)
H13	1.2022	1.1453	0.4895	0.041*
C14	1.0563 (2)	1.0014 (2)	0.38061 (18)	0.0287 (5)
H14	1.0213	1.0503	0.3342	0.034*
C15	0.8605 (2)	0.58748 (19)	0.07894 (15)	0.0237 (4)
C16	1.0115 (2)	0.6651 (2)	0.11952 (15)	0.0238 (4)
C17	1.0748 (3)	0.4960 (2)	0.15386 (19)	0.0367 (6)
H17	1.1473	0.4608	0.1803	0.044*
C18	0.9262 (3)	0.4196 (2)	0.11519 (19)	0.0359 (6)
H18	0.9000	0.3341	0.1169	0.043*
C19	0.7352 (2)	0.6281 (2)	0.02701 (16)	0.0255 (5)
C20	0.6387 (3)	0.5709 (2)	−0.06908 (18)	0.0372 (6)
H20	0.6503	0.5048	−0.1000	0.045*
C21	0.5258 (3)	0.6114 (3)	−0.11883 (19)	0.0451 (7)
H21	0.4610	0.5743	−0.1844	0.054*
C22	0.5088 (3)	0.7067 (3)	−0.0719 (2)	0.0423 (7)

H22	0.4329	0.7360	−0.1050	0.051*
C23	0.6045 (2)	0.7585 (2)	0.02450 (19)	0.0333 (5)
H23	0.5919	0.8228	0.0570	0.040*
C24	1.0708 (2)	0.8015 (2)	0.11849 (16)	0.0250 (4)
C25	1.1870 (3)	0.8527 (2)	0.08430 (19)	0.0367 (6)
H25	1.2285	0.8019	0.0619	0.044*
C26	1.2419 (3)	0.9791 (3)	0.0832 (2)	0.0444 (7)
H26	1.3218	1.0151	0.0609	0.053*
C27	1.1782 (3)	1.0513 (2)	0.1153 (2)	0.0409 (6)
H27	1.2132	1.1372	0.1143	0.049*
C28	1.0624 (3)	0.9964 (2)	0.14890 (18)	0.0329 (5)
H28	1.0180	1.0456	0.1701	0.039*
N9	0.7053 (3)	0.0811 (2)	0.17671 (19)	0.0425 (5)
O1	0.6818 (3)	0.1389 (3)	0.23751 (18)	0.0810 (8)
O2	0.7579 (3)	0.0012 (2)	0.1979 (3)	0.1035 (12)
O3	0.6834 (5)	0.1134 (4)	0.0945 (2)	0.1297 (15)
N10	0.2051 (3)	0.3037 (2)	0.3109 (2)	0.0463 (6)
O4	0.2775 (3)	0.3406 (2)	0.40190 (18)	0.0636 (6)
O5	0.0679 (2)	0.25210 (19)	0.2792 (2)	0.0688 (7)
O6	0.2740 (3)	0.3221 (2)	0.2514 (2)	0.0695 (7)
N11	0.3636 (4)	−0.0592 (4)	0.3507 (3)	0.0822 (10)
C29	0.4999 (4)	0.1768 (4)	0.3903 (4)	0.0813 (12)
H29A	0.5525	0.2046	0.3445	0.122*
H29B	0.5707	0.1988	0.4587	0.122*
H29C	0.4278	0.2163	0.3828	0.122*
C30	0.4232 (4)	0.0439 (4)	0.3679 (3)	0.0623 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01659 (9)	0.01646 (9)	0.02448 (9)	0.00547 (6)	0.00380 (6)	0.00146 (6)
N1	0.0380 (11)	0.0216 (9)	0.0258 (10)	0.0080 (8)	0.0102 (8)	0.0027 (7)
N2	0.0320 (10)	0.0327 (11)	0.0268 (10)	0.0149 (9)	0.0090 (8)	0.0052 (8)
N3	0.0180 (8)	0.0207 (9)	0.0288 (9)	0.0041 (7)	0.0052 (7)	−0.0062 (7)
N4	0.0180 (8)	0.0204 (9)	0.0275 (9)	0.0045 (7)	0.0087 (7)	−0.0026 (7)
N5	0.0367 (11)	0.0227 (10)	0.0338 (11)	0.0063 (8)	0.0145 (9)	0.0021 (8)
N6	0.0303 (10)	0.0342 (11)	0.0344 (11)	0.0151 (9)	0.0132 (9)	0.0068 (9)
N7	0.0195 (9)	0.0219 (9)	0.0266 (9)	0.0043 (7)	0.0034 (7)	0.0074 (7)
N8	0.0222 (9)	0.0218 (9)	0.0230 (9)	0.0048 (7)	0.0041 (7)	0.0042 (7)
C1	0.0288 (11)	0.0206 (10)	0.0178 (10)	0.0072 (9)	0.0088 (8)	0.0019 (8)
C2	0.0267 (11)	0.0248 (11)	0.0172 (10)	0.0080 (9)	0.0083 (8)	0.0019 (8)
C3	0.0437 (14)	0.0345 (13)	0.0334 (13)	0.0228 (11)	0.0158 (11)	0.0110 (10)
C4	0.0504 (15)	0.0231 (11)	0.0302 (12)	0.0167 (11)	0.0144 (11)	0.0075 (9)
C5	0.0227 (10)	0.0209 (10)	0.0273 (11)	0.0011 (8)	0.0079 (9)	−0.0064 (9)
C6	0.0346 (13)	0.0308 (13)	0.0443 (15)	0.0004 (10)	0.0210 (11)	−0.0030 (11)
C7	0.0325 (14)	0.0420 (16)	0.0607 (18)	−0.0029 (12)	0.0246 (13)	−0.0120 (14)
C8	0.0197 (12)	0.0479 (16)	0.0647 (19)	0.0058 (11)	0.0126 (12)	−0.0196 (14)
C9	0.0212 (11)	0.0314 (13)	0.0450 (14)	0.0087 (10)	0.0042 (10)	−0.0107 (11)

C10	0.0178 (10)	0.0246 (11)	0.0265 (11)	0.0056 (8)	0.0090 (8)	−0.0013 (9)
C11	0.0244 (11)	0.0354 (13)	0.0266 (11)	0.0074 (10)	0.0058 (9)	−0.0034 (10)
C12	0.0239 (11)	0.0386 (14)	0.0344 (13)	0.0028 (10)	0.0050 (10)	−0.0142 (11)
C13	0.0261 (12)	0.0242 (11)	0.0454 (14)	−0.0001 (9)	0.0146 (11)	−0.0131 (10)
C14	0.0247 (11)	0.0201 (11)	0.0405 (13)	0.0044 (9)	0.0149 (10)	−0.0029 (9)
C15	0.0280 (11)	0.0210 (10)	0.0204 (10)	0.0057 (9)	0.0102 (9)	0.0017 (8)
C16	0.0268 (11)	0.0255 (11)	0.0194 (10)	0.0083 (9)	0.0103 (9)	0.0033 (8)
C17	0.0438 (14)	0.0375 (14)	0.0409 (14)	0.0238 (12)	0.0208 (12)	0.0103 (11)
C18	0.0488 (15)	0.0243 (12)	0.0417 (14)	0.0159 (11)	0.0224 (12)	0.0051 (10)
C19	0.0217 (10)	0.0218 (10)	0.0234 (11)	−0.0001 (8)	0.0047 (9)	0.0039 (8)
C20	0.0319 (13)	0.0374 (14)	0.0262 (12)	−0.0010 (11)	0.0048 (10)	−0.0002 (10)
C21	0.0296 (13)	0.0485 (16)	0.0281 (13)	−0.0054 (12)	−0.0055 (10)	0.0073 (12)
C22	0.0210 (12)	0.0460 (15)	0.0435 (15)	0.0036 (11)	−0.0006 (11)	0.0237 (13)
C23	0.0238 (11)	0.0300 (12)	0.0419 (14)	0.0092 (10)	0.0067 (10)	0.0152 (10)
C24	0.0236 (10)	0.0242 (11)	0.0206 (10)	0.0035 (9)	0.0052 (8)	0.0024 (8)
C25	0.0375 (13)	0.0353 (13)	0.0361 (13)	0.0060 (11)	0.0195 (11)	0.0033 (11)
C26	0.0458 (15)	0.0380 (14)	0.0452 (15)	−0.0009 (12)	0.0280 (13)	0.0082 (12)
C27	0.0478 (15)	0.0254 (12)	0.0403 (14)	0.0003 (11)	0.0176 (12)	0.0103 (11)
C28	0.0362 (13)	0.0222 (11)	0.0325 (12)	0.0061 (10)	0.0074 (10)	0.0061 (9)
N9	0.0446 (13)	0.0276 (11)	0.0576 (15)	0.0164 (10)	0.0179 (11)	0.0038 (10)
O1	0.0879 (19)	0.124 (2)	0.0508 (14)	0.0659 (18)	0.0220 (13)	0.0027 (15)
O2	0.0523 (14)	0.0291 (11)	0.209 (4)	0.0242 (11)	0.0119 (18)	0.0110 (16)
O3	0.202 (4)	0.184 (4)	0.071 (2)	0.125 (4)	0.075 (2)	0.043 (2)
N10	0.0505 (15)	0.0224 (11)	0.0667 (17)	0.0219 (10)	0.0132 (13)	0.0075 (11)
O4	0.0732 (16)	0.0563 (14)	0.0582 (14)	0.0345 (12)	0.0090 (12)	−0.0004 (11)
O5	0.0470 (13)	0.0366 (11)	0.110 (2)	0.0152 (10)	0.0123 (13)	0.0097 (12)
O6	0.0829 (17)	0.0708 (16)	0.0788 (17)	0.0431 (14)	0.0430 (15)	0.0216 (13)
N11	0.093 (3)	0.092 (3)	0.079 (2)	0.052 (2)	0.034 (2)	0.008 (2)
C29	0.060 (2)	0.084 (3)	0.115 (3)	0.046 (2)	0.030 (2)	0.015 (2)
C30	0.061 (2)	0.087 (3)	0.059 (2)	0.052 (2)	0.0209 (17)	0.008 (2)

Geometric parameters (Å, º)

Pd1—N7	2.0170 (18)	C12—H12	0.9400
Pd1—N8	2.0178 (18)	C13—C14	1.383 (3)
Pd1—N4	2.0257 (17)	C13—H13	0.9400
Pd1—N3	2.0286 (19)	C14—H14	0.9400
N1—C4	1.333 (3)	C15—C16	1.403 (3)
N1—C1	1.345 (3)	C15—C19	1.485 (3)
N2—C3	1.329 (3)	C16—C24	1.493 (3)
N2—C2	1.344 (3)	C17—C18	1.380 (4)
N3—C9	1.344 (3)	C17—H17	0.9400
N3—C5	1.351 (3)	C18—H18	0.9400
N4—C14	1.347 (3)	C19—C20	1.388 (3)
N4—C10	1.347 (3)	C20—C21	1.376 (4)
N5—C18	1.325 (3)	C20—H20	0.9400
N5—C15	1.346 (3)	C21—C22	1.373 (4)
N6—C17	1.331 (3)	C21—H21	0.9400

N6—C16	1.341 (3)	C22—C23	1.376 (4)
N7—C19	1.349 (3)	C22—H22	0.9400
N7—C23	1.350 (3)	C23—H23	0.9400
N8—C24	1.349 (3)	C24—C25	1.381 (3)
N8—C28	1.349 (3)	C25—C26	1.384 (4)
C1—C2	1.400 (3)	C25—H25	0.9400
C1—C5	1.490 (3)	C26—C27	1.375 (4)
C2—C10	1.490 (3)	C26—H26	0.9400
C3—C4	1.381 (4)	C27—C28	1.380 (4)
C3—H3	0.9400	C27—H27	0.9400
C4—H4	0.9400	C28—H28	0.9400
C5—C6	1.385 (3)	N9—O3	1.211 (4)
C6—C7	1.392 (4)	N9—O2	1.218 (3)
C6—H6	0.9400	N9—O1	1.219 (3)
C7—C8	1.367 (4)	N10—O5	1.235 (3)
C7—H7	0.9400	N10—O4	1.245 (3)
C8—C9	1.383 (4)	N10—O6	1.248 (3)
C8—H8	0.9400	N11—C30	1.123 (5)
C9—H9	0.9400	C29—C30	1.446 (6)
C10—C11	1.384 (3)	C29—H29A	0.9700
C11—C12	1.380 (3)	C29—H29B	0.9700
C11—H11	0.9400	C29—H29C	0.9700
C12—C13	1.372 (4)		

N7—Pd1—N8	85.98 (7)	C14—C13—H13	120.4
N7—Pd1—N4	177.88 (7)	N4—C14—C13	121.8 (2)
N8—Pd1—N4	92.86 (7)	N4—C14—H14	119.1
N7—Pd1—N3	94.14 (7)	C13—C14—H14	119.1
N8—Pd1—N3	178.89 (7)	N5—C15—C16	120.7 (2)
N4—Pd1—N3	86.99 (7)	N5—C15—C19	113.75 (19)
C4—N1—C1	116.7 (2)	C16—C15—C19	125.20 (19)
C3—N2—C2	116.9 (2)	N6—C16—C15	120.9 (2)
C9—N3—C5	119.0 (2)	N6—C16—C24	113.55 (19)
C9—N3—Pd1	121.60 (17)	C15—C16—C24	125.26 (19)
C5—N3—Pd1	119.40 (14)	N6—C17—C18	121.9 (2)
C14—N4—C10	119.34 (19)	N6—C17—H17	119.0
C14—N4—Pd1	119.98 (15)	C18—C17—H17	119.0
C10—N4—Pd1	120.63 (14)	N5—C18—C17	121.6 (2)
C18—N5—C15	117.5 (2)	N5—C18—H18	119.2
C17—N6—C16	117.2 (2)	C17—C18—H18	119.2
C19—N7—C23	119.2 (2)	N7—C19—C20	120.7 (2)
C19—N7—Pd1	120.11 (14)	N7—C19—C15	119.79 (18)
C23—N7—Pd1	120.68 (17)	C20—C19—C15	119.5 (2)
C24—N8—C28	119.8 (2)	C21—C20—C19	119.6 (3)
C24—N8—Pd1	120.24 (14)	C21—C20—H20	120.2
C28—N8—Pd1	119.90 (16)	C19—C20—H20	120.2
N1—C1—C2	121.4 (2)	C22—C21—C20	119.5 (2)
N1—C1—C5	113.28 (19)	C22—C21—H21	120.3

C2—C1—C5	125.07 (19)	C20—C21—H21	120.3
N2—C2—C1	120.8 (2)	C21—C22—C23	119.0 (2)
N2—C2—C10	113.82 (18)	C21—C22—H22	120.5
C1—C2—C10	125.21 (19)	C23—C22—H22	120.5
N2—C3—C4	122.2 (2)	N7—C23—C22	122.0 (2)
N2—C3—H3	118.9	N7—C23—H23	119.0
C4—C3—H3	118.9	C22—C23—H23	119.0
N1—C4—C3	121.7 (2)	N8—C24—C25	120.7 (2)
N1—C4—H4	119.2	N8—C24—C16	119.67 (19)
C3—C4—H4	119.2	C25—C24—C16	119.6 (2)
N3—C5—C6	121.3 (2)	C24—C25—C26	119.7 (2)
N3—C5—C1	119.16 (19)	C24—C25—H25	120.2
C6—C5—C1	119.5 (2)	C26—C25—H25	120.2
C5—C6—C7	119.1 (3)	C27—C26—C25	119.1 (2)
C5—C6—H6	120.4	C27—C26—H26	120.4
C7—C6—H6	120.4	C25—C26—H26	120.4
C8—C7—C6	119.2 (3)	C26—C27—C28	119.3 (2)
C8—C7—H7	120.4	C26—C27—H27	120.3
C6—C7—H7	120.4	C28—C27—H27	120.3
C7—C8—C9	119.3 (3)	N8—C28—C27	121.3 (2)
C7—C8—H8	120.4	N8—C28—H28	119.3
C9—C8—H8	120.4	C27—C28—H28	119.3
N3—C9—C8	122.1 (3)	O3—N9—O2	120.7 (3)
N3—C9—H9	119.0	O3—N9—O1	116.2 (3)
C8—C9—H9	119.0	O2—N9—O1	122.9 (3)
N4—C10—C11	120.8 (2)	O5—N10—O4	121.2 (3)
N4—C10—C2	119.52 (18)	O5—N10—O6	120.2 (3)
C11—C10—C2	119.6 (2)	O4—N10—O6	118.6 (3)
C12—C11—C10	119.8 (2)	C30—C29—H29A	109.5
C12—C11—H11	120.1	C30—C29—H29B	109.5
C10—C11—H11	120.1	H29A—C29—H29B	109.5
C13—C12—C11	119.1 (2)	C30—C29—H29C	109.5
C13—C12—H12	120.4	H29A—C29—H29C	109.5
C11—C12—H12	120.4	H29B—C29—H29C	109.5
C12—C13—C14	119.1 (2)	N11—C30—C29	179.9 (5)
C12—C13—H13	120.4		

C4—N1—C1—C2	−0.6 (3)	C18—N5—C15—C16	2.3 (3)
C4—N1—C1—C5	−175.51 (19)	C18—N5—C15—C19	176.1 (2)
C3—N2—C2—C1	3.9 (3)	C17—N6—C16—C15	−3.0 (3)
C3—N2—C2—C10	179.72 (19)	C17—N6—C16—C24	−177.0 (2)
N1—C1—C2—N2	−3.6 (3)	N5—C15—C16—N6	0.8 (3)
C5—C1—C2—N2	170.7 (2)	C19—C15—C16—N6	−172.3 (2)
N1—C1—C2—C10	−178.84 (19)	N5—C15—C16—C24	174.0 (2)
C5—C1—C2—C10	−4.5 (3)	C19—C15—C16—C24	1.0 (3)
C2—N2—C3—C4	−0.4 (3)	C16—N6—C17—C18	2.1 (4)
C1—N1—C4—C3	4.1 (3)	C15—N5—C18—C17	−3.2 (4)
N2—C3—C4—N1	−3.8 (4)	N6—C17—C18—N5	1.0 (4)

C9—N3—C5—C6	2.2 (3)	C23—N7—C19—C20	−2.4 (3)
Pd1—N3—C5—C6	−177.06 (17)	Pd1—N7—C19—C20	179.11 (16)
C9—N3—C5—C1	179.91 (19)	C23—N7—C19—C15	177.89 (19)
Pd1—N3—C5—C1	0.7 (3)	Pd1—N7—C19—C15	−0.6 (3)
N1—C1—C5—N3	−127.1 (2)	N5—C15—C19—N7	131.2 (2)
C2—C1—C5—N3	58.2 (3)	C16—C15—C19—N7	−55.3 (3)
N1—C1—C5—C6	50.6 (3)	N5—C15—C19—C20	−48.5 (3)
C2—C1—C5—C6	−124.1 (2)	C16—C15—C19—C20	125.0 (2)
N3—C5—C6—C7	−2.3 (3)	N7—C19—C20—C21	2.7 (3)
C1—C5—C6—C7	179.9 (2)	C15—C19—C20—C21	−177.6 (2)
C5—C6—C7—C8	0.5 (4)	C19—C20—C21—C22	−1.1 (4)
C6—C7—C8—C9	1.3 (4)	C20—C21—C22—C23	−0.6 (4)
C5—N3—C9—C8	−0.2 (3)	C19—N7—C23—C22	0.6 (3)
Pd1—N3—C9—C8	179.01 (18)	Pd1—N7—C23—C22	179.05 (17)
C7—C8—C9—N3	−1.6 (4)	C21—C22—C23—N7	0.9 (4)
C14—N4—C10—C11	0.1 (3)	C28—N8—C24—C25	2.4 (3)
Pd1—N4—C10—C11	177.58 (16)	Pd1—N8—C24—C25	−174.04 (17)
C14—N4—C10—C2	−177.47 (19)	C28—N8—C24—C16	−178.37 (19)
Pd1—N4—C10—C2	0.0 (3)	Pd1—N8—C24—C16	5.2 (3)
N2—C2—C10—N4	131.5 (2)	N6—C16—C24—N8	−134.9 (2)
C1—C2—C10—N4	−52.9 (3)	C15—C16—C24—N8	51.4 (3)
N2—C2—C10—C11	−46.0 (3)	N6—C16—C24—C25	44.3 (3)
C1—C2—C10—C11	129.5 (2)	C15—C16—C24—C25	−129.4 (2)
N4—C10—C11—C12	−1.5 (3)	N8—C24—C25—C26	−0.9 (4)
C2—C10—C11—C12	176.1 (2)	C16—C24—C25—C26	179.9 (2)
C10—C11—C12—C13	1.1 (4)	C24—C25—C26—C27	−0.8 (4)
C11—C12—C13—C14	0.5 (4)	C25—C26—C27—C28	0.8 (4)
C10—N4—C14—C13	1.7 (3)	C24—N8—C28—C27	−2.4 (3)
Pd1—N4—C14—C13	−175.86 (17)	Pd1—N8—C28—C27	174.09 (18)
C12—C13—C14—N4	−2.0 (3)	C26—C27—C28—N8	0.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{i}	0.94	2.43	3.344 (3)	164
C4—H4···O1	0.94	2.51	3.330 (4)	146
C9—H9···O2^{ii}	0.94	2.40	3.113 (4)	133
C14—H14···O5^{iii}	0.94	2.43	3.257 (3)	147
C17—H17···O6^{i}	0.94	2.43	3.343 (3)	164
C22—H22···O3^{iv}	0.94	2.45	3.273 (5)	146
C23—H23···O2^{ii}	0.94	2.54	3.275 (4)	136
C29—H29*A*···O1	0.97	2.58	3.405 (5)	144
C29—H29*C*···O4	0.97	2.51	3.459 (4)	167

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