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Synthesis and crystal structure of a Pd^{II} complex of *ortho*-xylylenebis(pyridyltriazole)

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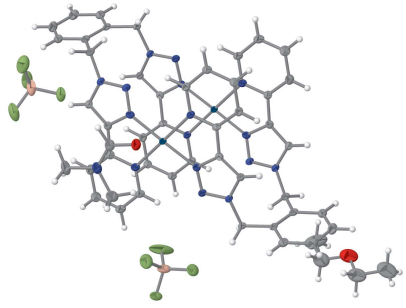
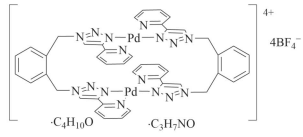
Structural data: full structural data are available from iucrdata.iucr.org

A tetradentate ligand, namely, *ortho*-xylylenebis(pyridyltriazole), *o*-xpt, was synthesized using the 'click' method and complexed with $Pd(BF_4)_2$. In the title complex, bis{μ-1,1′-(*o*-xylylene)bis[4-(pyridin-2-yl)triazole]-κN^3:$N^{3'}$}dipalladium(II) tetrakis(tetrafluoridoborate)–dimethylformamide–diethyl ether (1/2/1), as the BF_4 salt, and including dimethylformamide and diethyl ether solvent molecules, with stoichiometry $[Pd_2(C_{22}H_{18}N_8)_2](BF_4)_4{\cdot}2C_3H_7NO{\cdot}C_4H_{10}O$, the Pd complex and the disordered diethyl ether molecule lie on inversion centers. The ligand coordinates to the Pd^{II} centers with square-planar geometry, forming a dimeric macrocycle. The Pd···Pd separation in the complex $[Pd_2(o\text{-xpt})_2]^{4+}$ cation is 3.6184 (4) Å. In the crystal, the complex molecules are stacked along the *b* axis, with π–π interactions between the pyridyltriazole ligands of two molecules.

3D view



Chemical scheme



Structure description

The self-assembly of polydentate ligands with transition-metal ions to create functional metal–organic supramolecules has been of great interest in recent years. In particular, the complexation of 2-pyridyl-1,2,3-triazole chelating pockets with transition-metal ions has intensified due to the ease of synthesis of the ligands through the copper-catalyzed azide–alkyne cycloaddition (CuAAC) reaction (Crowley & McMorran, 2012). We and others have studied the complexation of *ortho*-, *meta*-, and *para*-xylylene-bridged pyridyltriazole tetradentate ligand with Cu^{II} (Pokharel *et al.*, 2013, 2014), Ni^{II} (Pokharel *et al.*, 2020*b*), Fe^{II} (Vellas *et al.*, 2013), Ag^{I} (Gower & Crowley, 2010), and Cu^{I} (Zhao *et al.*, 2013). We have recently studied the crystal structure of 1,1-bis(pyridyltriazoylmethyl)ferrocene and its complexation with Cu^{I} (Pokharel *et al.*, 2020*a*). As an extension of this work, we were also interested in studying the complexation of *ortho*-xylylene-

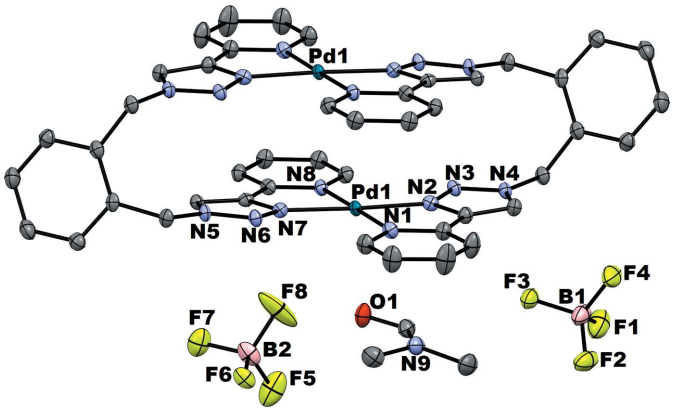


Figure 1
The molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level, and H atoms and disordered solvent molecules have been omitted for clarity.

bis(pyridyltriazole), *o*-xpt, with Pd^{II}. Herein, we report the synthesis and crystal structure of the title compound.

The structure of the title compound consists of the cationic Pd^{II} complex $[Pd_2(o\text{-xpt})_2]^{4+}$ lying on an inversion center, two BF_4^- anions in general positions, a dimethylformamide solvent molecule in a general position and a diethyl ether solvent molecule disordered about an inversion center (Fig. 1). In the complex, two Pd^{II} cations are coordinated by two tetradentate *o*-xpt ligands, giving a dimeric macrocycle. The two pyridyltriazole units are coordinated to each metal center in a *trans* fashion. The Pd^{II} centers are tetracoordinated in a square-planar geometry defined by four (N1, N2, N7 and N8) atoms of two pyridyltriazole moieties. The N—Pd—N chelating angles are N1—Pd1—N2 = 79.46 (8)° and N7—Pd1—N8 = 79.75 (8)°. The N(py)—Pd bonds [py is pyridine; average 2.055 (2) Å] are slightly longer than N(trz)—Pd bonds [trz is triazole; average 1.995 (2) Å], suggesting the triazolium

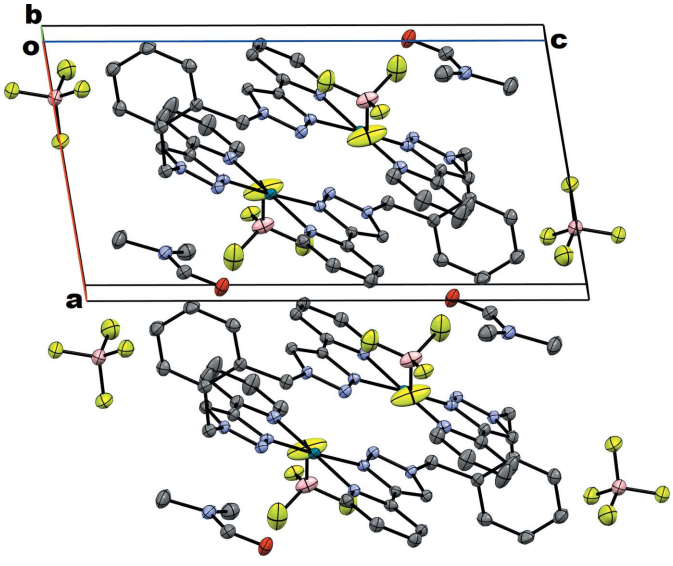


Figure 2
A view along the *b* axis of the crystal packing of the title compound. Disordered diethyl ether molecules have been omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Pd_2(C_{22}H_{18}N_8)_2](BF_4)_4\cdot 2C_3H_7NO\cdot C_4H_{10}O$
M_r	1569.24
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	90
a, b, c (Å)	8.3546 (4), 12.4468 (5), 15.4504 (6)
α, β, γ (°)	85.540 (2), 79.660 (2), 76.997 (2)
V (Å^3)	1538.86 (11)
Z	1
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.68
Crystal size (mm)	0.08 × 0.04 × 0.01
Data collection	
Diffractometer	Bruker Kappa APEXII CCD DUO
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.765, 0.945
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17544, 5427, 4983
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.076, 1.03
No. of reflections	5427
No. of parameters	456
No. of restraints	34
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.68, −0.41

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020), and *publCIF* (Westrip, 2010).

N atom coordinates more strongly to the Pd center than the pyridyl N atom of the ligand. These values are typical for the reported mononuclear Pd^{II} complex of pyridyltriazole ligands (Kilpin *et al.*, 2011). The Pd···Pd separation in the complex is 3.6184 (4) Å. Two phenylene moieties in the complex are in an antiparallel orientation, with an interplanar separation of 7.802 Å.

In the crystal packing, the pyridyltriazole units between two adjacent molecules are associated in a head-to-tail arrangement (the electron-rich pyridyl group of one molecule stacks over the electron-deficient triazole group of the other molecule) with an average interplanar distance of 3.364 Å, indicating π–π interaction between the molecules; this is shown along the *b* axis in Fig. 2.

Synthesis and crystallization

To a stirred solution of $[Pd(CH_3CN)_4]BF_4$ (0.112 mg, 0.253 mol) in acetonitrile (5 ml), *o*-xpt (0.100 g, 0.253 mmol) in acetonitrile (5 ml) was added dropwise. The solution was stirred for 1 h at room temperature. The volatiles were removed *in vacuo*. The residue was washed with dichloromethane (2 ml), followed by methanol (2 ml), and dried under vacuum to give $[Pd_2(o\text{-xpt})_2](BF_4)_4$ (0.126 mg, 74%) as a pale-yellow solid. Crystals suitable for X-ray analysis were obtained by slow vapor diffusion of diethyl ether into a dimethyl-

formamide (DMF) solution of the complex at room temperature. Our attempts to obtain a clean ^{1}H NMR spectrum in DMSO-d_6 were not successful, possibly due to the labile nature of the complex in solution. High resolution ESI–MS analysis showed a monocationic signal at m/z 1255.1478 {calculated 1255.1540 for $[Pd_2(o\text{-xpt})_2(BF_4)_4]^+$}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were located in difference maps and thereafter treated as riding in geometrically idealized positions, with C—H = 0.95 Å for Csp^2, 0.98 Å for methyl, and 0.99 Å for CH_2. U_{iso}(H) values were assigned as $1.2U_{eq}$ for the attached atom (1.5 for methyl). A torsional parameter was refined for each methyl group, except for those of the diethyl ether molecule, which were staggered with respect to CH_2. The diethyl ether solvent molecule is disordered about an inversion center with two half-populated sites. A number of distance and displacement parameter restraints were necessary to model the disorder.

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full crystallographic data

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Synthesis and crystal structure of a Pd^{II} complex of *ortho*-xylylenebis(pyridyltriazole)

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Bis{μ-1,1′-(*o*-xylylene)bis[4-(pyridin-2-yl)triazole]-κN^3:$N^{3'}$}dipalladium(II) tetrakis(tetrafluoridoborate)–dimethylformamide–diethyl ether (1/2/1)

Crystal data

$[Pd_2(C_{22}H_{18}N_8)_2](BF_4)_4{\cdot}2C_3H_7NO{\cdot}C_4H_{10}O$
M_r = 1569.24
Triclinic, $P\overline{1}$
a = 8.3546 (4) Å
b = 12.4468 (5) Å
c = 15.4504 (6) Å
α = 85.540 (2)°
β = 79.660 (2)°
γ = 76.997 (2)°
V = 1538.86 (11) Å^3
Z = 1
$F(000)$ = 790
D_x = 1.693 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 7868 reflections
θ = 2.9–68.3°
μ = 5.68 mm^{-1}
T = 90 K
Fragment, pale yellow
0.08 × 0.04 × 0.01 mm

Data collection

Bruker Kappa APEXII CCD DUO diffractometer
Radiation source: IμS microfocus
QUAZAR multilayer optics monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.765, T_{max} = 0.945
17544 measured reflections
5427 independent reflections
4983 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 68.5°, θ_{min} = 3.7°
h = −9→10
k = −14→10
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.03
5427 reflections
456 parameters
34 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 1.022P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pd1	0.62296 (2)	0.54481 (2)	0.40085 (2)	0.01235 (8)	
N1	0.4910 (3)	0.67202 (18)	0.33215 (15)	0.0177 (5)	
N2	0.5621 (3)	0.46128 (17)	0.31114 (14)	0.0154 (4)	
N3	0.5861 (3)	0.35595 (17)	0.29813 (14)	0.0154 (4)	
N4	0.5089 (3)	0.34974 (17)	0.23042 (14)	0.0156 (4)	
N5	0.2946 (3)	0.26548 (17)	0.41317 (14)	0.0145 (4)	
N6	0.3668 (3)	0.26845 (17)	0.48321 (14)	0.0157 (4)	
N7	0.3247 (3)	0.37183 (17)	0.50545 (14)	0.0144 (4)	
N8	0.2416 (3)	0.58271 (17)	0.53220 (14)	0.0152 (4)	
C1	0.4641 (4)	0.7791 (2)	0.34815 (19)	0.0218 (6)	
H1	0.506819	0.800711	0.395483	0.026*	
C2	0.3757 (4)	0.8589 (2)	0.2975 (2)	0.0310 (7)	
H2	0.358914	0.934618	0.309918	0.037*	
C3	0.3116 (5)	0.8291 (3)	0.2290 (2)	0.0378 (8)	
H3	0.248716	0.883448	0.194498	0.045*	
C4	0.3410 (4)	0.7178 (2)	0.2113 (2)	0.0294 (7)	
H4	0.299455	0.694820	0.164041	0.035*	
C5	0.4312 (3)	0.6413 (2)	0.26347 (18)	0.0189 (5)	
C6	0.4704 (3)	0.5227 (2)	0.25314 (17)	0.0173 (5)	
C7	0.4363 (3)	0.4500 (2)	0.20031 (17)	0.0175 (5)	
H7	0.375086	0.466634	0.152977	0.021*	
C8	0.5148 (3)	0.2393 (2)	0.19970 (18)	0.0176 (5)	
H8A	0.580939	0.182775	0.235508	0.021*	
H8B	0.572049	0.233842	0.137765	0.021*	
C9	0.3437 (3)	0.2151 (2)	0.20577 (17)	0.0171 (5)	
C10	0.2720 (4)	0.2300 (2)	0.12980 (18)	0.0212 (6)	
H10	0.329220	0.257654	0.077049	0.025*	
C11	0.1185 (4)	0.2050 (2)	0.12995 (19)	0.0255 (6)	
H11	0.070824	0.216010	0.077702	0.031*	
C12	0.0348 (4)	0.1642 (2)	0.20627 (19)	0.0252 (6)	
H12	−0.069897	0.146220	0.206446	0.030*	
C13	0.1041 (3)	0.1494 (2)	0.28270 (18)	0.0206 (6)	
H13	0.046137	0.121030	0.334933	0.025*	
C14	0.2570 (3)	0.1754 (2)	0.28398 (17)	0.0161 (5)	
C15	0.3232 (3)	0.1588 (2)	0.36990 (17)	0.0171 (5)	
H15A	0.266954	0.107126	0.409490	0.021*	
H15B	0.444077	0.125712	0.358676	0.021*	
C16	0.2068 (3)	0.3655 (2)	0.39066 (16)	0.0146 (5)	
H16	0.144232	0.383836	0.343930	0.018*	
C17	0.2283 (3)	0.4345 (2)	0.45040 (16)	0.0148 (5)	
C18	0.1818 (3)	0.5523 (2)	0.46399 (17)	0.0154 (5)	
C19	0.0907 (3)	0.6280 (2)	0.41110 (17)	0.0176 (5)	
H19	0.049619	0.604355	0.364009	0.021*	
C20	0.0605 (3)	0.7394 (2)	0.42825 (18)	0.0198 (6)	
H20	−0.000657	0.793352	0.392719	0.024*	

C21	0.1214 (3)	0.7704 (2)	0.49825 (18)	0.0198 (5)	
H21	0.102035	0.846091	0.511181	0.024*	
C22	0.2102 (3)	0.6906 (2)	0.54896 (17)	0.0178 (5)	
H22	0.250380	0.712569	0.597095	0.021*	
B1	0.7437 (5)	0.3502 (4)	−0.0041 (2)	0.0341 (8)	
F1	0.8450 (3)	0.2509 (2)	−0.03601 (14)	0.0497 (5)	
F2	0.7818 (2)	0.43622 (19)	−0.06116 (12)	0.0442 (5)	
F3	0.7724 (2)	0.36416 (16)	0.07958 (11)	0.0324 (4)	
F4	0.5762 (2)	0.34747 (19)	−0.00012 (12)	0.0429 (5)	
B2	0.7718 (4)	0.9939 (3)	0.3743 (3)	0.0305 (8)	
F5	0.8893 (3)	0.94186 (17)	0.30537 (14)	0.0536 (6)	
F6	0.7324 (2)	1.10683 (13)	0.35316 (12)	0.0273 (4)	
F7	0.8434 (3)	0.97815 (15)	0.45036 (12)	0.0394 (5)	
F8	0.6308 (3)	0.95332 (18)	0.3871 (2)	0.0773 (9)	
O1	0.9776 (3)	0.49882 (17)	0.27263 (13)	0.0280 (5)	
N9	0.8519 (3)	0.6141 (2)	0.17162 (16)	0.0248 (5)	
C23	0.9211 (3)	0.5157 (2)	0.20272 (19)	0.0239 (6)	
H23	0.927928	0.453656	0.169054	0.029*	
C24	0.8557 (4)	0.7145 (3)	0.2135 (2)	0.0314 (7)	
H24A	0.857946	0.698513	0.276396	0.047*	
H24B	0.756191	0.771129	0.205856	0.047*	
H24C	0.955517	0.741219	0.186200	0.047*	
C25	0.8014 (4)	0.6276 (3)	0.0849 (2)	0.0364 (8)	
H25A	0.876235	0.665880	0.044140	0.055*	
H25B	0.686950	0.671119	0.089651	0.055*	
H25C	0.807063	0.554943	0.062787	0.055*	
O2	0.4535 (11)	0.9884 (7)	1.0054 (7)	0.067 (3)	0.5
C26	0.3717 (19)	1.0268 (16)	0.9327 (11)	0.072 (4)	0.5
H26A	0.441392	0.995410	0.877955	0.086*	0.5
H26B	0.353021	1.108211	0.926463	0.086*	0.5
C27	0.2032 (17)	0.9910 (10)	0.9481 (10)	0.094 (4)	0.5
H27A	0.145357	1.017146	0.898066	0.141*	0.5
H27B	0.222622	0.910310	0.953778	0.141*	0.5
H27C	0.134518	1.022771	1.002139	0.141*	0.5
C28	0.6073 (17)	1.0284 (14)	0.9992 (12)	0.067 (3)	0.5
H28A	0.580069	1.110043	0.999418	0.081*	0.5
H28B	0.680609	1.006214	0.942838	0.081*	0.5
C29	0.699 (2)	0.9832 (15)	1.0748 (12)	0.086 (5)	0.5
H29A	0.801333	1.011668	1.068363	0.129*	0.5
H29B	0.628024	1.006203	1.130644	0.129*	0.5
H29C	0.728516	0.902423	1.074091	0.129*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01319 (11)	0.00994 (11)	0.01434 (11)	−0.00127 (7)	−0.00446 (7)	−0.00152 (7)
N1	0.0181 (11)	0.0147 (11)	0.0203 (11)	−0.0029 (9)	−0.0039 (9)	−0.0016 (9)
N2	0.0137 (10)	0.0129 (10)	0.0187 (11)	−0.0014 (8)	−0.0024 (9)	−0.0003 (8)

N3	0.0146 (10)	0.0140 (10)	0.0183 (11)	−0.0027 (8)	−0.0038 (9)	−0.0033 (8)
N4	0.0164 (11)	0.0157 (11)	0.0156 (10)	−0.0035 (9)	−0.0041 (9)	−0.0039 (8)
N5	0.0162 (11)	0.0131 (10)	0.0154 (10)	−0.0024 (8)	−0.0052 (8)	−0.0034 (8)
N6	0.0168 (11)	0.0130 (10)	0.0181 (11)	−0.0023 (8)	−0.0055 (9)	−0.0023 (8)
N7	0.0144 (10)	0.0134 (10)	0.0150 (10)	−0.0019 (8)	−0.0024 (8)	−0.0006 (8)
N8	0.0155 (11)	0.0145 (10)	0.0161 (10)	−0.0026 (8)	−0.0030 (9)	−0.0035 (8)
C1	0.0275 (15)	0.0146 (13)	0.0239 (14)	−0.0032 (11)	−0.0067 (12)	−0.0026 (11)
C2	0.0466 (19)	0.0138 (13)	0.0343 (17)	−0.0009 (13)	−0.0178 (15)	−0.0021 (12)
C3	0.059 (2)	0.0178 (15)	0.0375 (18)	0.0055 (14)	−0.0276 (17)	−0.0004 (13)
C4	0.0412 (18)	0.0213 (14)	0.0272 (16)	0.0004 (13)	−0.0188 (14)	−0.0006 (12)
C5	0.0213 (13)	0.0167 (13)	0.0187 (13)	−0.0022 (11)	−0.0056 (11)	−0.0014 (10)
C6	0.0177 (13)	0.0168 (13)	0.0174 (13)	−0.0028 (10)	−0.0048 (10)	0.0002 (10)
C7	0.0192 (13)	0.0175 (13)	0.0160 (12)	−0.0027 (10)	−0.0049 (10)	−0.0020 (10)
C8	0.0187 (13)	0.0141 (12)	0.0205 (13)	−0.0021 (10)	−0.0044 (11)	−0.0045 (10)
C9	0.0178 (13)	0.0129 (12)	0.0208 (13)	−0.0013 (10)	−0.0043 (10)	−0.0050 (10)
C10	0.0257 (14)	0.0183 (13)	0.0200 (13)	−0.0042 (11)	−0.0048 (11)	−0.0027 (10)
C11	0.0239 (15)	0.0297 (15)	0.0252 (15)	−0.0044 (12)	−0.0107 (12)	−0.0032 (12)
C12	0.0189 (14)	0.0300 (15)	0.0298 (15)	−0.0071 (12)	−0.0073 (12)	−0.0061 (12)
C13	0.0198 (13)	0.0194 (13)	0.0226 (14)	−0.0040 (11)	−0.0019 (11)	−0.0049 (11)
C14	0.0187 (13)	0.0112 (11)	0.0180 (13)	0.0009 (10)	−0.0055 (10)	−0.0056 (9)
C15	0.0224 (13)	0.0109 (12)	0.0182 (13)	−0.0014 (10)	−0.0055 (11)	−0.0030 (10)
C16	0.0143 (12)	0.0143 (12)	0.0154 (12)	−0.0024 (10)	−0.0034 (10)	−0.0009 (9)
C17	0.0128 (12)	0.0150 (12)	0.0150 (12)	−0.0010 (10)	−0.0009 (10)	−0.0002 (9)
C18	0.0148 (12)	0.0118 (12)	0.0185 (13)	−0.0007 (10)	−0.0010 (10)	−0.0045 (10)
C19	0.0170 (13)	0.0187 (13)	0.0169 (13)	−0.0011 (10)	−0.0045 (10)	−0.0024 (10)
C20	0.0224 (14)	0.0150 (13)	0.0209 (13)	0.0009 (11)	−0.0068 (11)	−0.0009 (10)
C21	0.0232 (14)	0.0139 (12)	0.0217 (14)	−0.0015 (10)	−0.0046 (11)	−0.0018 (10)
C22	0.0180 (13)	0.0162 (13)	0.0182 (13)	−0.0015 (10)	−0.0017 (10)	−0.0044 (10)
B1	0.0245 (18)	0.057 (2)	0.0206 (17)	−0.0070 (16)	−0.0061 (14)	0.0010 (16)
F1	0.0433 (12)	0.0655 (14)	0.0374 (11)	−0.0002 (10)	−0.0085 (9)	−0.0133 (10)
F2	0.0301 (10)	0.0731 (15)	0.0282 (10)	−0.0117 (10)	−0.0081 (8)	0.0160 (9)
F3	0.0284 (9)	0.0488 (11)	0.0214 (9)	−0.0099 (8)	−0.0073 (7)	0.0014 (8)
F4	0.0256 (10)	0.0762 (15)	0.0305 (10)	−0.0159 (9)	−0.0090 (8)	0.0007 (9)
B2	0.0278 (18)	0.0158 (15)	0.050 (2)	−0.0031 (13)	−0.0145 (16)	0.0013 (14)
F5	0.0783 (16)	0.0320 (11)	0.0404 (11)	0.0168 (10)	−0.0169 (11)	−0.0069 (9)
F6	0.0243 (8)	0.0179 (8)	0.0408 (10)	−0.0040 (7)	−0.0110 (7)	0.0029 (7)
F7	0.0525 (12)	0.0270 (9)	0.0368 (10)	0.0019 (8)	−0.0169 (9)	0.0014 (8)
F8	0.0483 (14)	0.0306 (11)	0.166 (3)	−0.0230 (10)	−0.0454 (17)	0.0217 (15)
O1	0.0344 (12)	0.0262 (11)	0.0247 (11)	−0.0014 (9)	−0.0149 (9)	−0.0006 (8)
N9	0.0210 (12)	0.0313 (13)	0.0234 (12)	−0.0070 (10)	−0.0079 (10)	0.0047 (10)
C23	0.0200 (14)	0.0287 (15)	0.0234 (14)	−0.0045 (12)	−0.0060 (11)	0.0003 (12)
C24	0.0302 (16)	0.0278 (16)	0.0364 (17)	−0.0059 (13)	−0.0081 (14)	0.0030 (13)
C25	0.0362 (18)	0.050 (2)	0.0264 (16)	−0.0138 (15)	−0.0149 (14)	0.0119 (14)
O2	0.077 (7)	0.041 (4)	0.071 (3)	−0.004 (5)	0.013 (5)	−0.006 (3)
C26	0.091 (9)	0.048 (6)	0.067 (7)	0.000 (6)	−0.007 (6)	−0.004 (5)
C27	0.100 (9)	0.057 (7)	0.121 (11)	−0.028 (6)	0.021 (8)	−0.038 (7)
C28	0.077 (7)	0.041 (4)	0.071 (3)	−0.004 (5)	0.013 (5)	−0.006 (3)
C29	0.107 (13)	0.047 (8)	0.082 (9)	0.011 (9)	0.007 (10)	0.002 (6)

Geometric parameters (Å, º)

Pd1—N2	1.994 (2)	C16—C17	1.369 (4)
Pd1—N7^{i}	2.007 (2)	C16—H16	0.9500
Pd1—N1	2.055 (2)	C17—C18	1.451 (4)
Pd1—N8^{i}	2.056 (2)	C18—C19	1.384 (4)
N1—C1	1.336 (4)	C19—C20	1.390 (4)
N1—C5	1.364 (3)	C19—H19	0.9500
N2—N3	1.307 (3)	C20—C21	1.389 (4)
N2—C6	1.360 (3)	C20—H20	0.9500
N3—N4	1.339 (3)	C21—C22	1.381 (4)
N4—C7	1.346 (3)	C21—H21	0.9500
N4—C8	1.477 (3)	C22—H22	0.9500
N5—N6	1.337 (3)	B1—F3	1.387 (4)
N5—C16	1.350 (3)	B1—F2	1.389 (4)
N5—C15	1.485 (3)	B1—F4	1.398 (4)
N6—N7	1.311 (3)	B1—F1	1.400 (5)
N7—C17	1.357 (3)	B2—F8	1.360 (4)
N8—C22	1.346 (3)	B2—F7	1.394 (4)
N8—C18	1.356 (3)	B2—F6	1.396 (4)
C1—C2	1.379 (4)	B2—F5	1.401 (5)
C1—H1	0.9500	O1—C23	1.240 (3)
C2—C3	1.379 (4)	N9—C23	1.325 (4)
C2—H2	0.9500	N9—C24	1.459 (4)
C3—C4	1.392 (4)	N9—C25	1.462 (4)
C3—H3	0.9500	C23—H23	0.9500
C4—C5	1.378 (4)	C24—H24A	0.9800
C4—H4	0.9500	C24—H24B	0.9800
C5—C6	1.453 (4)	C24—H24C	0.9800
C6—C7	1.372 (4)	C25—H25A	0.9800
C7—H7	0.9500	C25—H25B	0.9800
C8—C9	1.512 (4)	C25—H25C	0.9800
C8—H8A	0.9900	O2—C26	1.415 (14)
C8—H8B	0.9900	O2—C28	1.465 (12)
C9—C10	1.393 (4)	C26—C27	1.543 (14)
C9—C14	1.408 (4)	C26—H26A	0.9900
C10—C11	1.385 (4)	C26—H26B	0.9900
C10—H10	0.9500	C27—H27A	0.9800
C11—C12	1.381 (4)	C27—H27B	0.9800
C11—H11	0.9500	C27—H27C	0.9800
C12—C13	1.388 (4)	C28—C29	1.515 (16)
C12—H12	0.9500	C28—H28A	0.9900
C13—C14	1.390 (4)	C28—H28B	0.9900
C13—H13	0.9500	C29—H29A	0.9800
C14—C15	1.510 (3)	C29—H29B	0.9800
C15—H15A	0.9900	C29—H29C	0.9800
C15—H15B	0.9900		

N2—Pd1—N7^{i}	177.57 (8)	N5—C16—C17	104.4 (2)
N2—Pd1—N1	79.46 (8)	N5—C16—H16	127.8
N7^{i}—Pd1—N1	100.55 (8)	C17—C16—H16	127.8
N2—Pd1—N8^{i}	100.27 (8)	N7—C17—C16	107.1 (2)
N7^{i}—Pd1—N8^{i}	79.75 (8)	N7—C17—C18	116.8 (2)
N1—Pd1—N8^{i}	179.01 (9)	C16—C17—C18	136.0 (2)
C1—N1—C5	119.1 (2)	N8—C18—C19	122.4 (2)
C1—N1—Pd1	125.63 (18)	N8—C18—C17	113.5 (2)
C5—N1—Pd1	115.24 (17)	C19—C18—C17	124.0 (2)
N3—N2—C6	111.1 (2)	C18—C19—C20	118.7 (2)
N3—N2—Pd1	132.75 (17)	C18—C19—H19	120.7
C6—N2—Pd1	116.02 (17)	C20—C19—H19	120.7
N2—N3—N4	105.32 (19)	C21—C20—C19	118.8 (2)
N3—N4—C7	112.2 (2)	C21—C20—H20	120.6
N3—N4—C8	118.0 (2)	C19—C20—H20	120.6
C7—N4—C8	129.8 (2)	C22—C21—C20	119.6 (2)
N6—N5—C16	112.4 (2)	C22—C21—H21	120.2
N6—N5—C15	118.5 (2)	C20—C21—H21	120.2
C16—N5—C15	129.2 (2)	N8—C22—C21	121.9 (2)
N7—N6—N5	105.12 (19)	N8—C22—H22	119.0
N6—N7—C17	111.1 (2)	C21—C22—H22	119.0
N6—N7—Pd1^{i}	134.09 (16)	F3—B1—F2	110.5 (3)
C17—N7—Pd1^{i}	114.81 (17)	F3—B1—F4	109.4 (3)
C22—N8—C18	118.5 (2)	F2—B1—F4	109.3 (3)
C22—N8—Pd1^{i}	126.47 (17)	F3—B1—F1	109.2 (3)
C18—N8—Pd1^{i}	115.02 (16)	F2—B1—F1	108.6 (3)
N1—C1—C2	121.5 (3)	F4—B1—F1	109.7 (3)
N1—C1—H1	119.2	F8—B2—F7	110.6 (3)
C2—C1—H1	119.2	F8—B2—F6	109.4 (3)
C3—C2—C1	120.1 (3)	F7—B2—F6	108.7 (3)
C3—C2—H2	120.0	F8—B2—F5	111.1 (3)
C1—C2—H2	120.0	F7—B2—F5	108.4 (3)
C2—C3—C4	118.7 (3)	F6—B2—F5	108.5 (3)
C2—C3—H3	120.6	C23—N9—C24	120.9 (2)
C4—C3—H3	120.6	C23—N9—C25	121.0 (3)
C5—C4—C3	118.9 (3)	C24—N9—C25	116.9 (3)
C5—C4—H4	120.6	O1—C23—N9	124.7 (3)
C3—C4—H4	120.6	O1—C23—H23	117.7
N1—C5—C4	121.7 (2)	N9—C23—H23	117.7
N1—C5—C6	113.4 (2)	N9—C24—H24A	109.5
C4—C5—C6	124.9 (3)	N9—C24—H24B	109.5
N2—C6—C7	106.7 (2)	H24A—C24—H24B	109.5
N2—C6—C5	115.9 (2)	N9—C24—H24C	109.5
C7—C6—C5	137.4 (2)	H24A—C24—H24C	109.5
N4—C7—C6	104.7 (2)	H24B—C24—H24C	109.5
N4—C7—H7	127.7	N9—C25—H25A	109.5
C6—C7—H7	127.7	N9—C25—H25B	109.5
N4—C8—C9	112.7 (2)	H25A—C25—H25B	109.5

N4—C8—H8A	109.1	N9—C25—H25C	109.5
C9—C8—H8A	109.1	H25A—C25—H25C	109.5
N4—C8—H8B	109.1	H25B—C25—H25C	109.5
C9—C8—H8B	109.1	C26—O2—C28	111.7 (9)
H8A—C8—H8B	107.8	O2—C26—C27	108.8 (12)
C10—C9—C14	119.1 (2)	O2—C26—H26A	109.9
C10—C9—C8	118.1 (2)	C27—C26—H26A	109.9
C14—C9—C8	122.7 (2)	O2—C26—H26B	109.9
C11—C10—C9	121.0 (3)	C27—C26—H26B	109.9
C11—C10—H10	119.5	H26A—C26—H26B	108.3
C9—C10—H10	119.5	C26—C27—H27A	109.5
C12—C11—C10	119.8 (3)	C26—C27—H27B	109.5
C12—C11—H11	120.1	H27A—C27—H27B	109.5
C10—C11—H11	120.1	C26—C27—H27C	109.5
C11—C12—C13	119.9 (3)	H27A—C27—H27C	109.5
C11—C12—H12	120.1	H27B—C27—H27C	109.5
C13—C12—H12	120.1	O2—C28—C29	111.9 (12)
C12—C13—C14	121.0 (3)	O2—C28—H28A	109.2
C12—C13—H13	119.5	C29—C28—H28A	109.2
C14—C13—H13	119.5	O2—C28—H28B	109.2
C13—C14—C9	119.1 (2)	C29—C28—H28B	109.2
C13—C14—C15	118.0 (2)	H28A—C28—H28B	107.9
C9—C14—C15	122.9 (2)	C28—C29—H29A	109.5
N5—C15—C14	110.7 (2)	C28—C29—H29B	109.5
N5—C15—H15A	109.5	H29A—C29—H29B	109.5
C14—C15—H15A	109.5	C28—C29—H29C	109.5
N5—C15—H15B	109.5	H29A—C29—H29C	109.5
C14—C15—H15B	109.5	H29B—C29—H29C	109.5
H15A—C15—H15B	108.1		

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