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A dimer-to-dimer metal–metal linear aggregate from a nitrate-bridged *cis*-(2,2′:6′,2″-terpyridyl-κ^3N)palladium(II) cofacial dimer

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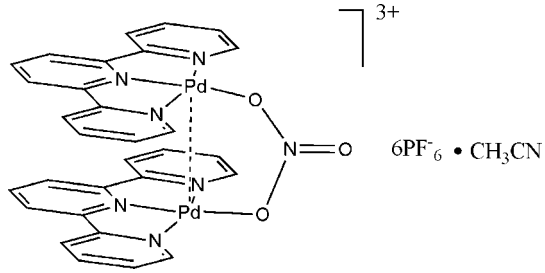
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.012 Å; R factor = 0.063; wR factor = 0.156; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, μ-nitrato-bis[(2,2′:6′,2″-terpyridyl-κ^3N)palladium(II)] hexakis(hexafluoridophosphate) acetonitrile solvate, $[Pd_2(C_{15}H_{11}N_3)_2NO_3]PF_6\cdot C_2H_3N$, contains two cationic dimers, $[Pd_2(C_{15}H_{11}N_3)_2NO_3]^{3+}$, six $(PF_6)^-$ anions and one CH_3CN solvent molecule. Each cationic dimer is built upon (μ-1,3-NO_3) bridging coordination to two *cis*-(2,2′:6′,2″-terpyridine)Pd^{II} units in a cofacial arrangement. The Pd atom is four-coordinated by a tridentate chelating 2,2′:6′,2″-terpyridine ligand and one bridging nitrate ion, to form a distorted square-planar geometry. The two dimers aggregate alternately along a linear chain *via* Pd···Pd interactions [intradimer, 3.09 (1) Å; interdimer, 3.33 (1) Å]. The dimer-to-dimer aggregates arrange in a zigzag orientation along the *b* axis through π–π interactions [centroid–centroid distances 3.521 (6)–3.894 (6)Å] between terpyridine ligands and weak intermolecular hydrogen bonds involving hexafluoridophosphate anions (C—H···F) and the solvent acetonitrile molecule (C—H···N).

Related literature

For related literature, see: Huang & Ma (2007); Mei & Huang (2007); Yu *et al.* (2001).



Experimental

Crystal data

$[Pd_2(C_{15}H_{11}N_3)_2NO_3]PF_6\cdot C_2H_3N$
M_r = 2393.57
Triclinic, $P\overline{1}$
a = 14.0633 (3) Å
b = 14.7277 (4) Å
c = 20.7043 (7) Å
α = 104.681 (4)°
β = 90.450 (1)°
γ = 102.226 (3)°
V = 4045.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 291 (2) K
0.32 × 0.28 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.71, T_{max} = 0.76
27513 measured reflections
17102 independent reflections
13353 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.156
S = 1.07
17102 reflections
1165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 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
C1—H1···F33	0.93	2.52	3.313 (12)	144
C3—H3···F13^{i}	0.93	2.47	3.402 (12)	176
C7—H7···F44^{ii}	0.93	2.45	3.223 (13)	140
C14—H14···F13	0.93	2.54	3.246 (11)	133
C16—H16···F33	0.93	2.32	3.051 (11)	135
C17—H17···F34^{iii}	0.93	2.46	3.291 (11)	150
C18—H18···F12^{i}	0.93	2.52	3.251 (12)	135
C22—H22···F43^{ii}	0.93	2.45	3.104 (11)	127
C24—H24···F52^{iv}	0.93	2.49	3.367 (9)	157
C30—H30···F15	0.93	2.39	3.192 (9)	145
C34—H34···N15^{i}	0.93	2.47	3.157 (16)	131
C38—H38···F71^{v}	0.93	2.33	3.159 (12)	148
C39—H39···F62^{vi}	0.93	2.54	3.474 (13)	179
C48—H48···F54^{i}	0.93	2.42	3.129 (11)	133
C52—H52···F31^{iii}	0.93	2.46	3.254 (11)	143
C54—H54···F11^{vi}	0.93	2.39	3.304 (10)	166
C60—H60···F51	0.93	2.34	3.188 (9)	151

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

Data collection: *RAPID-AUTO* (Rigaku, 1999); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *PLATON* (Spek, 2003); molecular graphics: *SHELXTL* (Sheldrick, 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: DN3057).

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supplementary materials

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A dimer-to-dimer metal-metal linear aggregate from a nitrate-bridged *cis*-(2,2':6',2''-terpyridyl-κ^3N)palladium(II) cofacial dimer

G.-Q. Mei, K.-L. Huang and H.-P. Huang

Comment

Recently, we have been interested in using 2,2':6',2''-terpyridine palladium (II) nitrate as a coordinative array in molecular self-assembly(Huang & Ma, 2007). To our knowledge, its solid structure is usually proposed as a monomer, and the crystal structure of its hexafluorophosphate has been reported (Mei & Huang, 2007). Herein we report the synthesis and structure of $\{cis$-[(2,2':6',2''-terpyridine)palladium(II)$]_2(\mu$-1,3-$NO_3)\}^{3+}$ (**I**). X-ray crystallographic analysis reveals that the dimerized *cis*-(2,2':6',2''-terpyridine)Pd(II) units aggregate into a dimer-to-dimer linear conformation through direct metal-metal interaction and π-π stacking between terpyridine ligands. A similar structure of $\{cis$-[(2,2'-bipyridine)palladium(II)$]_2(\mu$-1,3-$NO_3)_2\}^{2+}$ has been reported (Yu *et al.*, 2001).

In each dimeric cation of the title compound, $\{cis$-[(2,2':6',2''-terpyridine)palladium (II)$]_2\}(\mu$-1,3-$NO_3)\}^{3+}$, both Pd(II) atoms are coordinated by a 2,2':6',2''-terpyridine and bridged by nitrate anion in a cofacial arrangement. The geometry around Pd(II) is a distorted square-planar coordination, composed of three nitrogen atoms from the 2,2':6',2''-terpyridine and one oxygen atom from bridging nitrate (Fig. 1). The two bridged coordinated squares are arranged in an offset face-to-face stacking mode by a dihedral angle of 20°, conforming to an approximate π-π interaction. The resulting Pd···Pd distances (Pd1···Pd2 = 3.0939 (8) Å, Pd3···Pd4 = 3.0867 (8) Å) are significantly shorter than that in the 3,5-diphenyl pyrazolate bridged 2,2':6',2''-terpyridine palladinum complex $[Pd_2C_{45}H_{33}N_8](NO_3)_3$ (3.459 (1) Å)(Huang & Ma, 2007). The (μ-1,3-NO_3) nitrato-bridged N—O bonds are significantly shorter [1.27 (1)–1.32 (1) Å] than those of the uncoordination [1.51 (1)–1.52 (1) Å].

Interestingly, the two dimers aggregate alternatively along the linear chain consisting of the four Pd(II) atoms with Pd···Pd distances of 3.09 (1) Å (intradimer) and 3.33 (1)Å (interdimer), showing quite strong metal-metal interactions. The dimer-to-dimer aggregates arrange in a zigzag orientation along crystal axis *b* through π-π interactions and short contacts involving hexafluorophosphate anions (C—H···F) and the solvent acetonitrile molecule (C—H···N). The centroid-centroid contact between two pyridine rings of the terpyridine molecules and the angle between the ring-centroid vector and the ring normal to one of the pyridine planes in dimeric cation include: *Cg*1 (N1, C1 to C5)···*Cg*4 (N5, C16 to C20) 3.521 (6) Å, 15.0 (9)°; *Cg*2(N2, C6 to C10) ···*Cg*5(N5, C21 to C25) 3.894 (6) Å, 16.6 (1)°; *Cg*3(N3, C11 to C15)···*Cg*6(N7, C26 to C30) 3.624 (6) Å, 17.4 (1)°; *Cg*7(N8, C31 to C35)···*Cg*10(N12, C46 to C50) 3.521 (6) Å, 16.0 (4)°; *Cg*8(N9, C36 to C40)···*Cg*11(N13, C51 to C55) 3.894 (6) Å, 18.4 (6)°; *Cg*9(N10, C41 to C45)···*Cg*12(N14, C56 to C60) 3.624 (6) Å, 21.0 (2)°. While the centroid-centroid contact between two pyridine rings of the terpyridine molecules between the dimeric cations is *Cg*4···*Cg*10 3.732 (6) Å, and the angle between the ring-centroid vector and the ring normal to one of the pyridine planes 20.5 (3)°.

Among six hexafluorophosphate anions, two lie on inversion centre (P6, 1/2, 0, 0; P7, 1, 0, 0). The weak non-classical hydrogen bonds that connect cationic dimers, anions and acetonitrile solvent are detailed in Table 1.

Experimental

(2,2':6',2''-terpyridyl-κ^3N)dinitratopalladium (46.4 mg, 0.10 mmol) was dissolved in water (5 ml), and a twofold excess of potassium hexafluorophosphate was added, which resulted in the immediate deposition deep yellow microcrystals. The crystals were filtered, washed with a minimum amount of cold water and dried under vacuum (quantative yield, of 58.3 mg). Crystals were obtained by the vapor diffusion of diethyl ether into a 2 m*M* solution of in acetonitrile. ^{1}H NMR (400 MHz, [D_3] acetonitrile): δ 7.55 (2*H*, m, Ph—H), 8.03 (4*H*, m, Ph—H), 8.18 (6*H*, m, Ph—H), 8.37 (2*H*, m, Ph—H) p.p.m.

Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl) with U_{iso}(H) = 1.2U_{eq}(aromatic) or U_{iso}(H) = 1.5U_{eq}(methyl).

Some residual electron density were difficult to modelize and therefore, the SQUEEZE function of *PLATON* (Spek, 2003) was used to eliminate the contribution of the electron density in the solvent region from the intensity data, and the solvent-free model was employed for the final refinement.

There are two voids of about 15 Å^3 per unitl cell. *PLATON* estimated that each void contains 4.5 electrons which may correspond to roughly one water molecules within the cell.

Figures

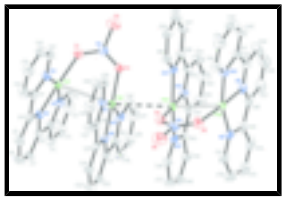


Fig. 1. The structures of independent cations title complexes, showing 30% probability displacement ellipsoids and the atom numbering scheme. H atoms have been omitted for clarity·The intermolecular Pd—Pd interaction is shown as dashed line.

μ-nitrato-bis[(2,2':6',2''-terpyridyl-κ3 N)palladium(II)] hexakis(hexafluorophosphate) acetonitrile solvate

Crystal data

$[Pd_2(C_{15}H_{11}N_3)_2NO_3]PF_6{\cdot}C_2H_3N$	Z = 2
M_r = 2393.57	F_{000} = 2340
Triclinic, $P\overline{1}$	D_x = 1.965 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.0633 (3) Å	Cell parameters from 683 reflections
b = 14.7277 (4) Å	θ = 1.0–27.5º
c = 20.7043 (7) Å	μ = 1.14 mm^{-1}
α = 104.681 (4)º	T = 291 (2) K
β = 90.450 (1)º	Block, yellow
γ = 102.226 (3)º	0.32 × 0.28 × 0.25 mm

V = 4045.6 (2) Å^3

Data collection

Rigaku R-AXIS RAPID IP diffractometer	17102 independent reflections
Radiation source: Rotating Anode	13353 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
T = 291(2) K	θ_{max} = 27.0º
Oscillation scans	θ_{min} = 1.0º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -17 \rightarrow 17$
T_{min} = 0.71, T_{max} = 0.76	$k = -18 \rightarrow 18$
27513 measured reflections	$l = 0 \rightarrow 26$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.156	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 15.4804P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
17102 reflections	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
1165 parameters	$\Delta\rho_{min}$ = −0.61 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > \sigma(F^2)$ 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	0.8441 (6)	0.2275 (5)	0.1255 (4)	0.0623 (18)
H1	0.8076	0.2349	0.0902	0.075*
C2	0.9424 (7)	0.2307 (6)	0.1205 (5)	0.082 (3)
H2	0.9713	0.2400	0.0818	0.099*

C3	0.9971 (7)	0.2206 (6)	0.1706 (6)	0.086 (3)
H3	1.0639	0.2254	0.1674	0.103*
C4	0.9523 (5)	0.2029 (6)	0.2273 (5)	0.070 (2)
H4	0.9884	0.1937	0.2620	0.084*
C5	0.8541 (5)	0.1994 (5)	0.2312 (4)	0.0542 (16)
C6	0.7971 (5)	0.1778 (4)	0.2868 (3)	0.0506 (15)
C7	0.8311 (6)	0.1654 (6)	0.3457 (4)	0.070 (2)
H7	0.8974	0.1714	0.3546	0.085*
C8	0.7660 (7)	0.1443 (7)	0.3908 (5)	0.085 (3)
H8	0.7887	0.1351	0.4304	0.101*
C9	0.6679 (7)	0.1363 (6)	0.3796 (4)	0.074 (2)
H9	0.6244	0.1223	0.4112	0.089*
C10	0.6351 (5)	0.1496 (5)	0.3197 (3)	0.0565 (16)
C11	0.5346 (5)	0.1491 (5)	0.2974 (3)	0.0555 (16)
C12	0.4539 (6)	0.1237 (7)	0.3313 (5)	0.080 (3)
H12	0.4598	0.1050	0.3706	0.096*
C13	0.3645 (6)	0.1267 (7)	0.3060 (5)	0.085 (3)
H13	0.3093	0.1116	0.3290	0.102*
C14	0.3557 (6)	0.1513 (7)	0.2477 (5)	0.082 (3)
H14	0.2948	0.1521	0.2303	0.099*
C15	0.4389 (5)	0.1753 (6)	0.2146 (4)	0.0642 (19)
H15	0.4331	0.1920	0.1746	0.077*
C16	0.8965 (6)	0.4625 (5)	0.1568 (4)	0.0606 (18)
H16	0.8495	0.4592	0.1239	0.073*
C17	0.9929 (7)	0.4792 (6)	0.1429 (5)	0.074 (2)
H17	1.0109	0.4873	0.1012	0.089*
C18	1.0616 (7)	0.4837 (6)	0.1907 (6)	0.086 (3)
H18	1.1272	0.4950	0.1818	0.103*
C19	1.0344 (6)	0.4714 (6)	0.2529 (5)	0.071 (2)
H19	1.0809	0.4729	0.2856	0.085*
C20	0.9358 (5)	0.4568 (5)	0.2648 (4)	0.0521 (15)
C21	0.8970 (5)	0.4443 (4)	0.3283 (3)	0.0493 (14)
C22	0.9466 (5)	0.4412 (6)	0.3856 (4)	0.0644 (19)
H22	1.0138	0.4470	0.3875	0.077*
C23	0.8935 (6)	0.4293 (6)	0.4391 (4)	0.070 (2)
H23	0.9257	0.4273	0.4780	0.084*
C24	0.7940 (6)	0.4202 (6)	0.4373 (3)	0.0649 (19)
H24	0.7593	0.4118	0.4742	0.078*
C25	0.7471 (5)	0.4238 (4)	0.3800 (3)	0.0473 (14)
C26	0.6412 (5)	0.4126 (5)	0.3665 (3)	0.0479 (14)
C27	0.5710 (6)	0.4027 (6)	0.4121 (4)	0.0658 (19)
H27	0.5888	0.4028	0.4555	0.079*
C28	0.4757 (6)	0.3927 (6)	0.3930 (4)	0.071 (2)
H28	0.4280	0.3844	0.4231	0.085*
C29	0.4499 (6)	0.3949 (6)	0.3298 (4)	0.067 (2)
H29	0.3850	0.3897	0.3169	0.080*
C30	0.5220 (5)	0.4051 (5)	0.2854 (3)	0.0530 (15)
H30	0.5048	0.4067	0.2423	0.064*
C31	0.8777 (6)	0.9041 (6)	0.3936 (4)	0.070 (2)

H31	0.8445	0.8834	0.4277	0.084*
C32	0.9779 (8)	0.9376 (7)	0.4015 (6)	0.098 (3)
H32	1.0118	0.9383	0.4404	0.117*
C33	1.0271 (7)	0.9702 (7)	0.3515 (8)	0.108 (4)
H33	1.0943	0.9939	0.3567	0.130*
C34	0.9757 (6)	0.9672 (6)	0.2939 (6)	0.090 (3)
H34	1.0080	0.9883	0.2595	0.108*
C35	0.8759 (5)	0.9327 (5)	0.2875 (4)	0.065 (2)
C36	0.8132 (6)	0.9311 (5)	0.2302 (4)	0.0627 (19)
C37	0.8396 (8)	0.9490 (7)	0.1688 (5)	0.090 (3)
H37	0.9049	0.9650	0.1600	0.108*
C38	0.7674 (9)	0.9425 (8)	0.1219 (6)	0.105 (4)
H38	0.7846	0.9559	0.0814	0.126*
C39	0.6713 (8)	0.9172 (8)	0.1328 (5)	0.093 (3)
H39	0.6234	0.9123	0.1000	0.112*
C40	0.6459 (6)	0.8988 (5)	0.1937 (4)	0.0621 (18)
C41	0.5476 (5)	0.8686 (5)	0.2152 (3)	0.0544 (16)
C42	0.4628 (7)	0.8680 (7)	0.1818 (4)	0.077 (2)
H42	0.4644	0.8851	0.1415	0.093*
C43	0.3746 (7)	0.8415 (8)	0.2090 (5)	0.089 (3)
H43	0.3163	0.8394	0.1865	0.107*
C44	0.3740 (6)	0.8187 (7)	0.2683 (5)	0.080 (2)
H44	0.3154	0.8023	0.2875	0.096*
C45	0.4602 (5)	0.8201 (6)	0.2998 (4)	0.0640 (19)
H45	0.4587	0.8032	0.3402	0.077*
C46	0.9099 (6)	0.6866 (5)	0.3674 (4)	0.0586 (17)
H46	0.8650	0.6723	0.3982	0.070*
C47	1.0085 (6)	0.7062 (6)	0.3856 (4)	0.072 (2)
H47	1.0293	0.7050	0.4281	0.086*
C48	1.0740 (6)	0.7271 (6)	0.3415 (5)	0.079 (2)
H48	1.1403	0.7414	0.3538	0.095*
C49	1.0431 (5)	0.7274 (6)	0.2777 (4)	0.068 (2)
H49	1.0881	0.7411	0.2470	0.081*
C50	0.9434 (5)	0.7066 (5)	0.2606 (3)	0.0497 (14)
C51	0.8998 (4)	0.7011 (5)	0.1951 (3)	0.0501 (15)
C52	0.9464 (6)	0.7191 (7)	0.1401 (4)	0.072 (2)
H52	1.0139	0.7390	0.1422	0.086*
C53	0.8923 (6)	0.7073 (8)	0.0823 (4)	0.086 (3)
H53	0.9236	0.7175	0.0445	0.104*
C54	0.7925 (6)	0.6806 (7)	0.0790 (4)	0.077 (2)
H54	0.7562	0.6729	0.0395	0.093*
C55	0.7468 (5)	0.6652 (5)	0.1354 (3)	0.0507 (15)
C56	0.6402 (5)	0.6389 (5)	0.1440 (3)	0.0515 (15)
C57	0.5688 (5)	0.6230 (6)	0.0938 (4)	0.0642 (19)
H57	0.5849	0.6283	0.0512	0.077*
C58	0.4731 (6)	0.5989 (6)	0.1088 (4)	0.074 (2)
H58	0.4235	0.5873	0.0758	0.089*
C59	0.4500 (5)	0.5917 (6)	0.1722 (4)	0.066 (2)
H59	0.3855	0.5752	0.1826	0.080*

C60	0.5254 (5)	0.6098 (5)	0.2195 (3)	0.0538 (15)
H60	0.5106	0.6054	0.2625	0.065*
C61	0.1844 (10)	0.9551 (11)	0.1525 (7)	0.131 (5)
C62	0.2378 (10)	0.9738 (11)	0.0963 (7)	0.136 (5)
H62A	0.3015	0.9607	0.0993	0.205*
H62B	0.2440	1.0400	0.0964	0.205*
H62C	0.2031	0.9332	0.0555	0.205*
F11	0.3301 (4)	0.3848 (5)	0.0682 (3)	0.119 (2)
F12	0.2561 (7)	0.3968 (8)	0.1639 (5)	0.197 (5)
F13	0.2405 (5)	0.2426 (7)	0.1524 (5)	0.166 (4)
F14	0.3120 (8)	0.2367 (7)	0.0574 (6)	0.206 (5)
F15	0.3859 (4)	0.3387 (6)	0.1503 (3)	0.130 (3)
F16	0.1809 (4)	0.2967 (6)	0.0747 (3)	0.129 (3)
F21	0.5986 (6)	0.0326 (7)	0.5747 (4)	0.149 (3)
F22	0.6604 (6)	−0.0001 (4)	0.4719 (3)	0.113 (2)
F23	0.8034 (6)	0.0203 (9)	0.5206 (4)	0.184 (4)
F24	0.7447 (6)	0.0528 (5)	0.6218 (3)	0.123 (2)
F25	0.7226 (8)	0.1334 (5)	0.5479 (4)	0.168 (4)
F26	0.6799 (8)	−0.0800 (5)	0.5458 (3)	0.162 (4)
F31	0.8351 (6)	0.3205 (10)	−0.1226 (4)	0.206 (5)
F32	0.7038 (5)	0.2858 (8)	−0.0701 (4)	0.183 (5)
F33	0.7890 (5)	0.3505 (8)	0.0223 (3)	0.174 (4)
F34	0.9127 (5)	0.4075 (7)	−0.0323 (4)	0.157 (3)
F35	0.7673 (8)	0.4243 (8)	−0.0488 (11)	0.304 (10)
F36	0.8546 (11)	0.2592 (9)	−0.0474 (9)	0.269 (8)
F41	0.8457 (6)	0.7797 (6)	0.5182 (4)	0.152 (3)
F42	0.7670 (5)	0.7115 (9)	0.5912 (4)	0.184 (4)
F43	0.8981 (8)	0.6827 (8)	0.6252 (5)	0.186 (4)
F44	0.9753 (6)	0.7548 (13)	0.5545 (6)	0.264 (8)
F45	0.8903 (11)	0.8221 (6)	0.6293 (5)	0.236 (6)
F46	0.8550 (13)	0.6419 (6)	0.5186 (5)	0.249 (7)
F51	0.4019 (4)	0.6030 (6)	0.3473 (4)	0.138 (3)
F52	0.3325 (4)	0.5410 (5)	0.4247 (3)	0.0992 (18)
F53	0.1941 (4)	0.5869 (6)	0.4045 (3)	0.116 (2)
F54	0.2658 (6)	0.6500 (8)	0.3285 (5)	0.199 (5)
F55	0.2626 (6)	0.4985 (7)	0.3237 (4)	0.153 (3)
F56	0.3341 (7)	0.6859 (6)	0.4324 (7)	0.214 (5)
F61	0.4833 (6)	0.0345 (5)	0.0762 (3)	0.127 (2)
F62	0.5061 (7)	0.1027 (4)	−0.0091 (4)	0.152 (3)
F63	0.6111 (4)	0.0318 (6)	0.0229 (4)	0.131 (2)
F71	0.9031 (6)	0.0317 (7)	0.0224 (5)	0.164 (3)
F72	1.0373 (8)	0.0383 (8)	0.0745 (4)	0.191 (4)
F73	1.0362 (9)	0.0982 (6)	−0.0120 (6)	0.227 (6)
N1	0.8006 (4)	0.2138 (4)	0.1805 (3)	0.0507 (12)
N2	0.7009 (4)	0.1692 (4)	0.2757 (3)	0.0467 (12)
N3	0.5274 (4)	0.1751 (4)	0.2388 (3)	0.0526 (13)
N4	0.6167 (4)	0.3392 (5)	0.1162 (3)	0.0549 (14)
N5	0.8685 (4)	0.4510 (4)	0.2155 (3)	0.0503 (12)
N6	0.7995 (3)	0.4362 (3)	0.3279 (2)	0.0421 (11)

N7	0.6158 (4)	0.4128 (4)	0.3030 (2)	0.0439 (11)
N8	0.8280 (4)	0.9010 (4)	0.3372 (3)	0.0567 (14)
N9	0.7176 (4)	0.9067 (4)	0.2396 (3)	0.0517 (13)
N10	0.5470 (4)	0.8447 (4)	0.2750 (3)	0.0511 (12)
N11	0.6422 (4)	0.7095 (5)	0.3970 (3)	0.0651 (16)
N12	0.8774 (4)	0.6877 (4)	0.3066 (3)	0.0492 (12)
N13	0.8014 (4)	0.6745 (4)	0.1907 (2)	0.0434 (11)
N14	0.6179 (4)	0.6333 (4)	0.2066 (2)	0.0455 (11)
N15	0.1438 (11)	0.9385 (13)	0.1956 (7)	0.198 (7)
O1	0.6131 (4)	0.2523 (4)	0.1226 (3)	0.0703 (14)
O2	0.5685 (5)	0.3518 (6)	0.0542 (3)	0.105 (2)
O3	0.6582 (3)	0.4170 (3)	0.1593 (2)	0.0505 (10)
O4	0.6716 (4)	0.6451 (3)	0.3534 (2)	0.0551 (11)
O5	0.6432 (4)	0.7971 (4)	0.3917 (3)	0.0757 (15)
O6	0.6025 (6)	0.6805 (6)	0.4584 (3)	0.117 (3)
P1	0.28359 (14)	0.31449 (18)	0.11135 (11)	0.0682 (5)
P2	0.70198 (19)	0.02723 (16)	0.54697 (10)	0.0701 (6)
P3	0.80942 (15)	0.3441 (2)	−0.05047 (11)	0.0729 (6)
P4	0.87092 (17)	0.73181 (17)	0.57193 (12)	0.0735 (6)
P5	0.29837 (15)	0.59521 (18)	0.37584 (12)	0.0693 (6)
P6	0.5000	0.0000	0.0000	0.0582 (6)
P7	1.0000	0.0000	0.0000	0.0977 (13)
Pd1	0.65777 (4)	0.20609 (3)	0.19879 (2)	0.04358 (12)
Pd2	0.73012 (3)	0.42735 (3)	0.24547 (2)	0.03875 (11)
Pd3	0.68166 (4)	0.85813 (3)	0.31629 (2)	0.04592 (12)
Pd4	0.73706 (3)	0.66080 (3)	0.27017 (2)	0.04043 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.075 (5)	0.055 (4)	0.058 (4)	0.016 (3)	0.021 (4)	0.015 (3)
C2	0.094 (7)	0.069 (5)	0.092 (6)	0.027 (5)	0.048 (6)	0.025 (5)
C3	0.065 (5)	0.069 (5)	0.123 (8)	0.016 (4)	0.030 (6)	0.020 (5)
C4	0.051 (4)	0.065 (5)	0.093 (6)	0.013 (3)	0.006 (4)	0.022 (4)
C5	0.059 (4)	0.042 (3)	0.062 (4)	0.010 (3)	0.004 (3)	0.014 (3)
C6	0.052 (4)	0.043 (3)	0.059 (4)	0.009 (3)	−0.003 (3)	0.019 (3)
C7	0.064 (5)	0.077 (5)	0.079 (5)	0.013 (4)	−0.011 (4)	0.040 (4)
C8	0.091 (7)	0.101 (7)	0.072 (5)	0.019 (5)	−0.012 (5)	0.043 (5)
C9	0.084 (6)	0.084 (6)	0.066 (5)	0.014 (4)	0.013 (4)	0.046 (4)
C10	0.066 (4)	0.056 (4)	0.056 (4)	0.012 (3)	0.009 (3)	0.030 (3)
C11	0.057 (4)	0.055 (4)	0.057 (4)	0.006 (3)	0.005 (3)	0.024 (3)
C12	0.069 (5)	0.102 (7)	0.086 (6)	0.017 (5)	0.026 (5)	0.057 (5)
C13	0.061 (5)	0.094 (7)	0.111 (7)	0.011 (4)	0.024 (5)	0.051 (6)
C14	0.049 (4)	0.093 (6)	0.111 (7)	0.010 (4)	0.000 (5)	0.043 (6)
C15	0.058 (4)	0.066 (5)	0.072 (5)	0.008 (3)	0.004 (4)	0.029 (4)
C16	0.069 (5)	0.057 (4)	0.051 (4)	0.006 (3)	0.016 (3)	0.011 (3)
C17	0.073 (5)	0.065 (5)	0.080 (5)	0.008 (4)	0.037 (5)	0.017 (4)
C18	0.055 (5)	0.070 (5)	0.124 (8)	0.009 (4)	0.038 (5)	0.012 (5)

C19	0.049 (4)	0.066 (5)	0.088 (6)	0.012 (3)	0.010 (4)	0.005 (4)
C20	0.038 (3)	0.048 (4)	0.064 (4)	0.005 (3)	0.006 (3)	0.006 (3)
C21	0.050 (4)	0.037 (3)	0.054 (4)	0.006 (3)	−0.007 (3)	0.002 (3)
C22	0.047 (4)	0.068 (5)	0.074 (5)	0.011 (3)	−0.013 (4)	0.013 (4)
C23	0.067 (5)	0.089 (6)	0.053 (4)	0.020 (4)	−0.016 (4)	0.018 (4)
C24	0.076 (5)	0.078 (5)	0.036 (3)	0.012 (4)	−0.007 (3)	0.012 (3)
C25	0.057 (4)	0.045 (3)	0.037 (3)	0.010 (3)	0.003 (3)	0.009 (2)
C26	0.052 (4)	0.052 (4)	0.043 (3)	0.018 (3)	0.009 (3)	0.014 (3)
C27	0.067 (5)	0.086 (5)	0.051 (4)	0.021 (4)	0.017 (4)	0.026 (4)
C28	0.062 (5)	0.091 (6)	0.073 (5)	0.028 (4)	0.032 (4)	0.036 (4)
C29	0.049 (4)	0.080 (5)	0.078 (5)	0.024 (4)	0.011 (4)	0.025 (4)
C30	0.044 (3)	0.064 (4)	0.056 (4)	0.016 (3)	0.004 (3)	0.022 (3)
C31	0.070 (5)	0.061 (5)	0.067 (5)	0.020 (4)	−0.017 (4)	−0.010 (4)
C32	0.077 (7)	0.075 (6)	0.121 (9)	0.024 (5)	−0.025 (6)	−0.016 (6)
C33	0.054 (6)	0.072 (6)	0.184 (13)	0.013 (5)	−0.007 (7)	0.009 (7)
C34	0.053 (5)	0.058 (5)	0.153 (10)	0.007 (4)	0.020 (6)	0.020 (5)
C35	0.053 (4)	0.042 (4)	0.095 (6)	0.009 (3)	0.017 (4)	0.011 (4)
C36	0.062 (4)	0.045 (4)	0.085 (5)	0.012 (3)	0.030 (4)	0.023 (4)
C37	0.090 (7)	0.089 (6)	0.106 (7)	0.021 (5)	0.055 (6)	0.052 (6)
C38	0.119 (9)	0.124 (9)	0.096 (7)	0.031 (7)	0.049 (7)	0.069 (7)
C39	0.110 (8)	0.118 (8)	0.081 (6)	0.041 (6)	0.034 (6)	0.064 (6)
C40	0.068 (5)	0.059 (4)	0.065 (4)	0.013 (3)	0.014 (4)	0.028 (4)
C41	0.054 (4)	0.063 (4)	0.047 (3)	0.011 (3)	0.004 (3)	0.016 (3)
C42	0.077 (6)	0.094 (6)	0.068 (5)	0.027 (5)	0.005 (4)	0.027 (5)
C43	0.057 (5)	0.110 (8)	0.095 (7)	0.022 (5)	−0.004 (5)	0.015 (6)
C44	0.055 (5)	0.099 (7)	0.082 (6)	0.015 (4)	0.016 (4)	0.018 (5)
C45	0.055 (4)	0.074 (5)	0.064 (4)	0.015 (4)	0.016 (4)	0.019 (4)
C46	0.066 (4)	0.056 (4)	0.052 (4)	0.012 (3)	−0.005 (3)	0.013 (3)
C47	0.071 (5)	0.067 (5)	0.074 (5)	0.023 (4)	−0.023 (4)	0.004 (4)
C48	0.054 (5)	0.071 (5)	0.104 (7)	0.012 (4)	−0.019 (5)	0.013 (5)
C49	0.046 (4)	0.064 (5)	0.089 (6)	0.020 (3)	−0.003 (4)	0.007 (4)
C50	0.043 (3)	0.055 (4)	0.051 (3)	0.014 (3)	0.005 (3)	0.010 (3)
C51	0.039 (3)	0.060 (4)	0.053 (4)	0.017 (3)	0.009 (3)	0.011 (3)
C52	0.045 (4)	0.108 (7)	0.066 (5)	0.020 (4)	0.024 (4)	0.026 (4)
C53	0.064 (5)	0.142 (9)	0.059 (5)	0.028 (5)	0.027 (4)	0.031 (5)
C54	0.073 (5)	0.114 (7)	0.046 (4)	0.018 (5)	0.007 (4)	0.024 (4)
C55	0.047 (4)	0.066 (4)	0.041 (3)	0.017 (3)	0.004 (3)	0.014 (3)
C56	0.055 (4)	0.058 (4)	0.045 (3)	0.017 (3)	−0.003 (3)	0.017 (3)
C57	0.058 (4)	0.085 (5)	0.051 (4)	0.012 (4)	−0.011 (3)	0.024 (4)
C58	0.060 (5)	0.090 (6)	0.071 (5)	0.008 (4)	−0.019 (4)	0.026 (4)
C59	0.035 (3)	0.076 (5)	0.086 (5)	0.000 (3)	−0.004 (3)	0.028 (4)
C60	0.047 (4)	0.058 (4)	0.054 (4)	0.004 (3)	0.003 (3)	0.018 (3)
C61	0.092 (8)	0.149 (12)	0.122 (10)	0.004 (8)	0.036 (8)	−0.001 (9)
C62	0.109 (10)	0.170 (13)	0.129 (11)	0.013 (9)	0.039 (8)	0.051 (10)
F11	0.087 (4)	0.168 (6)	0.110 (4)	−0.013 (4)	−0.021 (3)	0.082 (4)
F12	0.151 (7)	0.239 (11)	0.175 (8)	0.095 (7)	0.030 (6)	−0.041 (8)
F13	0.095 (5)	0.240 (10)	0.210 (8)	−0.005 (5)	−0.006 (5)	0.177 (8)
F14	0.203 (10)	0.135 (7)	0.239 (11)	0.043 (7)	0.072 (8)	−0.034 (7)
F15	0.060 (3)	0.229 (8)	0.119 (5)	0.012 (4)	−0.020 (3)	0.096 (5)

F16	0.061 (3)	0.208 (7)	0.125 (5)	−0.007 (4)	−0.022 (3)	0.085 (5)
F21	0.114 (5)	0.202 (8)	0.134 (6)	0.056 (5)	0.020 (5)	0.030 (6)
F22	0.193 (7)	0.080 (4)	0.064 (3)	0.027 (4)	−0.021 (4)	0.020 (3)
F23	0.127 (6)	0.325 (14)	0.115 (6)	0.103 (8)	0.037 (5)	0.038 (7)
F24	0.164 (6)	0.146 (6)	0.060 (3)	0.055 (5)	−0.002 (4)	0.012 (3)
F25	0.309 (12)	0.070 (4)	0.111 (5)	0.019 (5)	0.005 (6)	0.017 (4)
F26	0.319 (12)	0.077 (4)	0.097 (5)	0.043 (6)	0.030 (6)	0.035 (4)
F31	0.094 (5)	0.412 (17)	0.085 (5)	0.040 (7)	0.032 (4)	0.025 (7)
F32	0.071 (4)	0.304 (12)	0.100 (5)	−0.024 (5)	0.020 (4)	−0.024 (6)
F33	0.095 (5)	0.335 (13)	0.077 (4)	−0.001 (6)	0.004 (4)	0.066 (6)
F34	0.085 (4)	0.204 (8)	0.139 (6)	−0.046 (5)	0.015 (4)	0.028 (6)
F35	0.159 (9)	0.164 (10)	0.64 (3)	0.063 (8)	0.002 (14)	0.174 (15)
F36	0.276 (15)	0.214 (12)	0.41 (2)	0.133 (11)	0.162 (15)	0.183 (13)
F41	0.176 (7)	0.186 (8)	0.151 (6)	0.087 (6)	0.032 (6)	0.107 (6)
F42	0.084 (5)	0.335 (14)	0.149 (7)	0.035 (6)	0.004 (5)	0.105 (8)
F43	0.229 (10)	0.249 (11)	0.158 (7)	0.156 (9)	0.021 (7)	0.105 (8)
F44	0.078 (5)	0.54 (3)	0.200 (10)	0.030 (9)	0.008 (6)	0.174 (14)
F45	0.407 (19)	0.097 (6)	0.153 (8)	−0.014 (8)	0.026 (10)	−0.004 (6)
F46	0.47 (2)	0.097 (6)	0.157 (8)	0.072 (9)	0.027 (11)	−0.012 (6)
F51	0.073 (4)	0.206 (8)	0.187 (7)	0.053 (4)	0.067 (4)	0.124 (6)
F52	0.096 (4)	0.155 (5)	0.074 (3)	0.061 (4)	0.017 (3)	0.052 (3)
F53	0.070 (3)	0.205 (7)	0.106 (4)	0.060 (4)	0.032 (3)	0.076 (5)
F54	0.160 (7)	0.317 (12)	0.263 (11)	0.158 (8)	0.121 (7)	0.245 (10)
F55	0.125 (6)	0.196 (8)	0.105 (5)	0.051 (5)	−0.030 (4)	−0.029 (5)
F56	0.175 (9)	0.090 (5)	0.321 (14)	0.025 (5)	−0.007 (9)	−0.043 (7)
F61	0.162 (6)	0.137 (6)	0.062 (3)	0.017 (5)	0.024 (4)	0.006 (3)
F62	0.258 (10)	0.057 (3)	0.126 (5)	0.006 (4)	−0.064 (6)	0.024 (3)
F63	0.076 (4)	0.180 (7)	0.135 (6)	0.010 (4)	−0.008 (4)	0.052 (5)
F71	0.125 (6)	0.173 (8)	0.188 (8)	0.049 (5)	0.075 (6)	0.021 (6)
F72	0.230 (11)	0.221 (11)	0.119 (6)	0.103 (9)	0.015 (7)	−0.007 (7)
F73	0.296 (14)	0.102 (6)	0.278 (13)	0.015 (7)	0.149 (11)	0.063 (7)
N1	0.053 (3)	0.045 (3)	0.055 (3)	0.010 (2)	0.011 (3)	0.013 (2)
N2	0.051 (3)	0.046 (3)	0.049 (3)	0.012 (2)	0.003 (2)	0.024 (2)
N3	0.049 (3)	0.061 (3)	0.054 (3)	0.012 (2)	0.005 (2)	0.026 (3)
N4	0.054 (3)	0.073 (4)	0.046 (3)	0.022 (3)	0.012 (3)	0.023 (3)
N5	0.048 (3)	0.049 (3)	0.048 (3)	0.003 (2)	0.009 (2)	0.007 (2)
N6	0.040 (3)	0.044 (3)	0.038 (2)	0.007 (2)	−0.003 (2)	0.006 (2)
N7	0.041 (3)	0.051 (3)	0.042 (3)	0.015 (2)	0.006 (2)	0.012 (2)
N8	0.050 (3)	0.044 (3)	0.069 (4)	0.010 (2)	0.001 (3)	0.003 (3)
N9	0.052 (3)	0.046 (3)	0.061 (3)	0.010 (2)	0.018 (3)	0.022 (3)
N10	0.050 (3)	0.054 (3)	0.051 (3)	0.013 (2)	0.010 (2)	0.016 (2)
N11	0.055 (4)	0.087 (5)	0.052 (3)	0.004 (3)	−0.002 (3)	0.025 (3)
N12	0.049 (3)	0.043 (3)	0.050 (3)	0.011 (2)	−0.006 (2)	0.001 (2)
N13	0.040 (3)	0.051 (3)	0.038 (2)	0.011 (2)	0.008 (2)	0.010 (2)
N14	0.044 (3)	0.049 (3)	0.043 (3)	0.009 (2)	0.003 (2)	0.012 (2)
N15	0.155 (12)	0.246 (18)	0.142 (11)	−0.010 (11)	0.075 (10)	−0.001 (11)
O1	0.087 (4)	0.066 (3)	0.057 (3)	0.011 (3)	−0.006 (3)	0.021 (3)
O2	0.099 (5)	0.152 (7)	0.079 (4)	0.038 (5)	−0.006 (4)	0.050 (4)
O3	0.063 (3)	0.047 (2)	0.041 (2)	0.010 (2)	0.000 (2)	0.0133 (19)

O4	0.064 (3)	0.060 (3)	0.043 (2)	0.012 (2)	0.015 (2)	0.016 (2)
O5	0.091 (4)	0.079 (4)	0.058 (3)	0.016 (3)	0.014 (3)	0.022 (3)
O6	0.113 (6)	0.167 (8)	0.074 (4)	0.007 (5)	0.021 (4)	0.055 (5)
P1	0.0466 (10)	0.0995 (16)	0.0659 (12)	0.0147 (10)	0.0017 (9)	0.0360 (12)
P2	0.0977 (16)	0.0608 (12)	0.0550 (11)	0.0238 (11)	0.0108 (11)	0.0156 (9)
P3	0.0496 (11)	0.1117 (18)	0.0578 (11)	0.0066 (11)	0.0118 (9)	0.0319 (12)
P4	0.0654 (13)	0.0750 (14)	0.0806 (14)	0.0214 (10)	−0.0151 (11)	0.0168 (11)
P5	0.0532 (11)	0.0926 (16)	0.0769 (13)	0.0260 (10)	0.0190 (10)	0.0399 (12)
P6	0.0728 (17)	0.0480 (14)	0.0519 (14)	0.0096 (12)	0.0047 (12)	0.0130 (11)
P7	0.096 (3)	0.075 (2)	0.107 (3)	0.0043 (19)	0.050 (2)	0.008 (2)
Pd1	0.0495 (3)	0.0423 (2)	0.0410 (2)	0.00723 (19)	0.00250 (19)	0.01685 (19)
Pd2	0.0396 (2)	0.0424 (2)	0.0338 (2)	0.00792 (17)	0.00260 (17)	0.01008 (17)
Pd3	0.0478 (3)	0.0451 (3)	0.0434 (2)	0.0076 (2)	0.0087 (2)	0.0111 (2)
Pd4	0.0399 (2)	0.0444 (2)	0.0359 (2)	0.00804 (18)	0.00250 (18)	0.00956 (18)

Geometric parameters (Å, °)

C1—N1	1.337 (9)	C48—C49	1.389 (12)
C1—C2	1.379 (12)	C48—H48	0.9300
C1—H1	0.9300	C49—C50	1.392 (9)
C2—C3	1.343 (14)	C49—H49	0.9300
C2—H2	0.9300	C50—N12	1.373 (8)
C3—C4	1.392 (13)	C50—C51	1.460 (9)
C3—H3	0.9300	C51—N13	1.352 (8)
C4—C5	1.375 (10)	C51—C52	1.374 (10)
C4—H4	0.9300	C52—C53	1.366 (12)
C5—N1	1.372 (9)	C52—H52	0.9300
C5—C6	1.470 (9)	C53—C54	1.370 (12)
C6—N2	1.345 (8)	C53—H53	0.9300
C6—C7	1.376 (10)	C54—C55	1.383 (10)
C7—C8	1.358 (12)	C54—H54	0.9300
C7—H7	0.9300	C55—N13	1.335 (8)
C8—C9	1.373 (12)	C55—C56	1.490 (9)
C8—H8	0.9300	C56—N14	1.355 (8)
C9—C10	1.395 (10)	C56—C57	1.380 (9)
C9—H9	0.9300	C57—C58	1.376 (11)
C10—N2	1.341 (8)	C57—H57	0.9300
C10—C11	1.482 (10)	C58—C59	1.380 (11)
C11—N3	1.372 (8)	C58—H58	0.9300
C11—C12	1.372 (10)	C59—C60	1.373 (10)
C12—C13	1.373 (12)	C59—H59	0.9300
C12—H12	0.9300	C60—N14	1.321 (8)
C13—C14	1.356 (12)	C60—H60	0.9300
C13—H13	0.9300	C61—N15	1.115 (17)
C14—C15	1.387 (11)	C61—C62	1.443 (17)
C14—H14	0.9300	C62—H62A	0.9602
C15—N3	1.338 (9)	C62—H62B	0.9597
C15—H15	0.9300	C62—H62C	0.9608
C16—N5	1.322 (8)	F11—P1	1.579 (6)

C16—C17	1.372 (11)	F12—P1	1.529 (8)
C16—H16	0.9300	F13—P1	1.550 (6)
C17—C18	1.357 (13)	F14—P1	1.508 (8)
C17—H17	0.9300	F15—P1	1.570 (5)
C18—C19	1.392 (13)	F16—P1	1.567 (6)
C18—H18	0.9300	F21—P2	1.577 (8)
C19—C20	1.391 (10)	F22—P2	1.577 (5)
C19—H19	0.9300	F23—P2	1.546 (8)
C20—N5	1.361 (9)	F24—P2	1.581 (6)
C20—C21	1.466 (10)	F25—P2	1.524 (7)
C21—N6	1.351 (8)	F26—P2	1.537 (7)
C21—C22	1.388 (10)	F31—P3	1.511 (7)
C22—C23	1.369 (11)	F32—P3	1.543 (7)
C22—H22	0.9300	F33—P3	1.518 (7)
C23—C24	1.377 (11)	F34—P3	1.536 (6)
C23—H23	0.9300	F35—P3	1.421 (10)
C24—C25	1.371 (9)	F36—P3	1.533 (11)
C24—H24	0.9300	F41—P4	1.536 (7)
C25—N6	1.340 (8)	F42—P4	1.507 (8)
C25—C26	1.480 (9)	F43—P4	1.550 (7)
C26—N7	1.361 (8)	F44—P4	1.503 (9)
C26—C27	1.382 (9)	F45—P4	1.515 (9)
C27—C28	1.362 (11)	F46—P4	1.468 (9)
C27—H27	0.9300	F51—P5	1.568 (5)
C28—C29	1.364 (11)	F52—P5	1.567 (5)
C28—H28	0.9300	F53—P5	1.579 (5)
C29—C30	1.384 (10)	F54—P5	1.541 (6)
C29—H29	0.9300	F55—P5	1.535 (8)
C30—N7	1.340 (8)	F56—P5	1.523 (9)
C30—H30	0.9300	F61—P6	1.565 (5)
C31—N8	1.341 (10)	F62—P6	1.556 (6)
C31—C32	1.384 (13)	F63—P6	1.566 (6)
C31—H31	0.9300	F71—P7	1.568 (7)
C32—C33	1.380 (16)	F72—P7	1.547 (9)
C32—H32	0.9300	F73—P7	1.511 (8)
C33—C34	1.376 (16)	N1—Pd1	2.032 (5)
C33—H33	0.9300	N2—Pd1	1.939 (5)
C34—C35	1.382 (11)	N3—Pd1	2.029 (5)
C34—H34	0.9300	N4—O3	1.282 (7)
C35—N8	1.362 (10)	N4—O1	1.310 (7)
C35—C36	1.465 (12)	N4—O2	1.518 (8)
C36—N9	1.344 (9)	N5—Pd2	2.033 (5)
C36—C37	1.399 (11)	N6—Pd2	1.920 (5)
C37—C38	1.371 (15)	N7—Pd2	2.015 (5)
C37—H37	0.9300	N8—Pd3	2.029 (6)
C38—C39	1.361 (14)	N9—Pd3	1.930 (5)
C38—H38	0.9300	N10—Pd3	2.022 (6)
C39—C40	1.390 (10)	N11—O4	1.273 (8)
C39—H39	0.9300	N11—O5	1.320 (8)

C40—N9	1.346 (9)	N11—O6	1.515 (8)
C40—C41	1.468 (10)	N12—Pd4	2.029 (5)
C41—N10	1.370 (8)	N13—Pd4	1.919 (5)
C41—C42	1.371 (11)	N14—Pd4	2.027 (5)
C42—C43	1.388 (13)	O1—Pd1	2.014 (5)
C42—H42	0.9300	O3—Pd2	1.999 (4)
C43—C44	1.353 (13)	O4—Pd4	2.003 (4)
C43—H43	0.9300	O5—Pd3	2.014 (5)
C44—C45	1.366 (11)	P6—F62^{i}	1.556 (6)
C44—H44	0.9300	P6—F61^{i}	1.565 (5)
C45—N10	1.343 (9)	P6—F63^{i}	1.566 (6)
C45—H45	0.9300	P7—F73^{ii}	1.511 (8)
C46—N12	1.343 (8)	P7—F72^{ii}	1.547 (9)
C46—C47	1.383 (11)	P7—F71^{ii}	1.568 (7)
C46—H46	0.9300	Pd1—Pd2	3.0940 (6)
C47—C48	1.347 (13)	Pd3—Pd4	3.0868 (7)
C47—H47	0.9300		
N1—C1—C2	120.6 (8)	C5—N1—Pd1	113.2 (4)
N1—C1—H1	119.7	C10—N2—C6	123.4 (6)
C2—C1—H1	119.7	C10—N2—Pd1	118.1 (4)
C3—C2—C1	121.3 (8)	C6—N2—Pd1	117.8 (4)
C3—C2—H2	119.4	C15—N3—C11	118.4 (6)
C1—C2—H2	119.4	C15—N3—Pd1	128.5 (5)
C2—C3—C4	118.9 (8)	C11—N3—Pd1	113.1 (4)
C2—C3—H3	120.6	O3—N4—O1	124.7 (5)
C4—C3—H3	120.6	O3—N4—O2	115.8 (6)
C5—C4—C3	119.1 (8)	O1—N4—O2	119.5 (6)
C5—C4—H4	120.5	C16—N5—C20	120.2 (6)
C3—C4—H4	120.5	C16—N5—Pd2	127.5 (5)
N1—C5—C4	120.8 (7)	C20—N5—Pd2	112.2 (4)
N1—C5—C6	114.4 (6)	C25—N6—C21	123.4 (5)
C4—C5—C6	124.7 (7)	C25—N6—Pd2	117.8 (4)
N2—C6—C7	119.2 (7)	C21—N6—Pd2	118.4 (4)
N2—C6—C5	113.2 (6)	C30—N7—C26	119.2 (5)
C7—C6—C5	127.6 (7)	C30—N7—Pd2	127.3 (4)
C8—C7—C6	118.7 (8)	C26—N7—Pd2	113.5 (4)
C8—C7—H7	120.6	C31—N8—C35	119.9 (7)
C6—C7—H7	120.6	C31—N8—Pd3	127.3 (6)
C7—C8—C9	122.1 (8)	C35—N8—Pd3	112.7 (5)
C7—C8—H8	119.0	C36—N9—C40	124.0 (6)
C9—C8—H8	119.0	C36—N9—Pd3	117.6 (5)
C8—C9—C10	118.2 (7)	C40—N9—Pd3	117.4 (4)
C8—C9—H9	120.9	C45—N10—C41	117.7 (6)
C10—C9—H9	120.9	C45—N10—Pd3	128.6 (5)
N2—C10—C9	118.5 (7)	C41—N10—Pd3	113.6 (4)
N2—C10—C11	113.0 (6)	O4—N11—O5	124.9 (6)
C9—C10—C11	128.4 (7)	O4—N11—O6	116.0 (7)

N3—C11—C12	121.7 (7)	O5—N11—O6	119.1 (7)
N3—C11—C10	114.5 (6)	C46—N12—C50	119.3 (6)
C12—C11—C10	123.8 (7)	C46—N12—Pd4	127.8 (5)
C11—C12—C13	118.5 (8)	C50—N12—Pd4	112.9 (4)
C11—C12—H12	120.8	C55—N13—C51	123.2 (5)
C13—C12—H12	120.8	C55—N13—Pd4	118.5 (4)
C14—C13—C12	120.7 (8)	C51—N13—Pd4	118.1 (4)
C14—C13—H13	119.6	C60—N14—C56	119.1 (6)
C12—C13—H13	119.6	C60—N14—Pd4	127.7 (4)
C13—C14—C15	118.9 (8)	C56—N14—Pd4	113.2 (4)
C13—C14—H14	120.6	N4—O1—Pd1	131.5 (4)
C15—C14—H14	120.6	N4—O3—Pd2	126.5 (4)
N3—C15—C14	121.8 (7)	N11—O4—Pd4	126.9 (4)
N3—C15—H15	119.1	N11—O5—Pd3	130.4 (5)
C14—C15—H15	119.1	F14—P1—F12	177.1 (7)
N5—C16—C17	121.9 (8)	F14—P1—F13	92.4 (6)
N5—C16—H16	119.1	F12—P1—F13	90.5 (6)
C17—C16—H16	119.1	F14—P1—F16	91.5 (6)
C18—C17—C16	119.2 (8)	F12—P1—F16	88.1 (5)
C18—C17—H17	120.4	F13—P1—F16	89.8 (4)
C16—C17—H17	120.4	F14—P1—F15	91.7 (6)
C17—C18—C19	120.3 (8)	F12—P1—F15	88.6 (5)
C17—C18—H18	119.9	F13—P1—F15	91.5 (4)
C19—C18—H18	119.9	F16—P1—F15	176.5 (5)
C20—C19—C18	118.1 (8)	F14—P1—F11	85.5 (6)
C20—C19—H19	121.0	F12—P1—F11	91.7 (6)
C18—C19—H19	121.0	F13—P1—F11	177.7 (5)
N5—C20—C19	120.2 (7)	F16—P1—F11	91.2 (3)
N5—C20—C21	115.8 (5)	F15—P1—F11	87.7 (3)
C19—C20—C21	124.0 (7)	F25—P2—F26	179.3 (7)
N6—C21—C22	119.0 (6)	F25—P2—F23	90.1 (6)
N6—C21—C20	112.2 (6)	F26—P2—F23	90.5 (6)
C22—C21—C20	128.9 (6)	F25—P2—F21	90.9 (5)
C23—C22—C21	117.9 (7)	F26—P2—F21	88.5 (5)
C23—C22—H22	121.1	F23—P2—F21	178.8 (6)
C21—C22—H22	121.1	F25—P2—F22	89.7 (4)
C22—C23—C24	122.1 (7)	F26—P2—F22	89.9 (4)
C22—C23—H23	118.9	F23—P2—F22	88.1 (4)
C24—C23—H23	118.9	F21—P2—F22	92.6 (4)
C25—C24—C23	118.6 (7)	F25—P2—F24	91.2 (4)
C25—C24—H24	120.7	F26—P2—F24	89.2 (4)
C23—C24—H24	120.7	F23—P2—F24	91.2 (4)
N6—C25—C24	119.1 (6)	F21—P2—F24	88.2 (4)
N6—C25—C26	113.3 (5)	F22—P2—F24	178.8 (4)
C24—C25—C26	127.6 (6)	F35—P3—F31	99.8 (10)
N7—C26—C27	120.6 (6)	F35—P3—F33	90.8 (9)
N7—C26—C25	113.9 (5)	F31—P3—F33	169.3 (7)
C27—C26—C25	125.5 (6)	F35—P3—F36	176.4 (11)
C28—C27—C26	119.5 (7)	F31—P3—F36	83.7 (7)

C28—C27—H27	120.2	F33—P3—F36	85.7 (7)
C26—C27—H27	120.2	F35—P3—F34	92.9 (7)
C27—C28—C29	120.3 (7)	F31—P3—F34	88.1 (5)
C27—C28—H28	119.9	F33—P3—F34	92.9 (4)
C29—C28—H28	119.9	F36—P3—F34	86.6 (7)
C28—C29—C30	118.7 (7)	F35—P3—F32	83.6 (7)
C28—C29—H29	120.6	F31—P3—F32	91.2 (4)
C30—C29—H29	120.6	F33—P3—F32	88.5 (4)
N7—C30—C29	121.7 (6)	F36—P3—F32	96.9 (8)
N7—C30—H30	119.2	F34—P3—F32	176.3 (6)
C29—C30—H30	119.2	F46—P4—F44	89.1 (9)
N8—C31—C32	120.8 (10)	F46—P4—F42	92.7 (8)
N8—C31—H31	119.6	F44—P4—F42	178.2 (8)
C32—C31—H31	119.6	F46—P4—F45	176.8 (8)
C33—C32—C31	119.7 (11)	F44—P4—F45	90.1 (8)
C33—C32—H32	120.1	F42—P4—F45	88.1 (7)
C31—C32—H32	120.1	F46—P4—F41	86.8 (6)
C34—C33—C32	119.3 (10)	F44—P4—F41	87.5 (6)
C34—C33—H33	120.4	F42—P4—F41	92.7 (5)
C32—C33—H33	120.4	F45—P4—F41	96.3 (6)
C33—C34—C35	119.4 (10)	F46—P4—F43	92.5 (6)
C33—C34—H34	120.3	F44—P4—F43	91.5 (6)
C35—C34—H34	120.3	F42—P4—F43	88.3 (5)
N8—C35—C34	120.8 (9)	F45—P4—F43	84.4 (6)
N8—C35—C36	114.9 (6)	F41—P4—F43	178.8 (5)
C34—C35—C36	124.2 (9)	F56—P5—F55	174.7 (6)
N9—C36—C37	117.9 (8)	F56—P5—F54	93.8 (7)
N9—C36—C35	113.0 (6)	F55—P5—F54	91.3 (6)
C37—C36—C35	129.0 (8)	F56—P5—F52	85.4 (6)
C38—C37—C36	118.8 (9)	F55—P5—F52	89.6 (4)
C38—C37—H37	120.6	F54—P5—F52	179.1 (6)
C36—C37—H37	120.6	F56—P5—F51	91.8 (6)
C39—C38—C37	121.9 (9)	F55—P5—F51	89.5 (5)
C39—C38—H38	119.1	F54—P5—F51	91.8 (4)
C37—C38—H38	119.1	F52—P5—F51	88.0 (3)
C38—C39—C40	118.8 (10)	F56—P5—F53	88.4 (5)
C38—C39—H39	120.6	F55—P5—F53	90.4 (4)
C40—C39—H39	120.6	F54—P5—F53	88.4 (3)
N9—C40—C39	118.6 (8)	F52—P5—F53	91.9 (3)
N9—C40—C41	113.7 (6)	F51—P5—F53	179.8 (4)
C39—C40—C41	127.7 (8)	F62—P6—F62^{i}	180.0 (8)
N10—C41—C42	121.4 (7)	F62—P6—F61	91.6 (4)
N10—C41—C40	113.7 (6)	F62^{i}—P6—F61	88.4 (4)
C42—C41—C40	124.9 (7)	F62—P6—F61^{i}	88.4 (4)
C41—C42—C43	119.1 (8)	F62^{i}—P6—F61^{i}	91.6 (4)
C41—C42—H42	120.4	F61—P6—F61^{i}	180.0 (6)
C43—C42—H42	120.4	F62—P6—F63	88.0 (4)
C44—C43—C42	119.5 (9)	F62^{i}—P6—F63	92.0 (4)

C44—C43—H43	120.2	F61—P6—F63	85.2 (4)
C42—C43—H43	120.2	F61^{i}—P6—F63	94.8 (4)
C43—C44—C45	119.4 (8)	F62—P6—F63^{i}	92.0 (4)
C43—C44—H44	120.3	F62^{i}—P6—F63^{i}	88.0 (4)
C45—C44—H44	120.3	F61—P6—F63^{i}	94.8 (4)
N10—C45—C44	122.8 (8)	F61^{i}—P6—F63^{i}	85.2 (4)
N10—C45—H45	118.6	F63—P6—F63^{i}	180.0 (6)
C44—C45—H45	118.6	F73^{ii}—P7—F73	180.0 (9)
N12—C46—C47	121.7 (8)	F73^{ii}—P7—F72	88.6 (7)
N12—C46—H46	119.2	F73—P7—F72	91.4 (7)
C47—C46—H46	119.2	F73^{ii}—P7—F72^{ii}	91.4 (7)
C48—C47—C46	119.6 (8)	F73—P7—F72^{ii}	88.6 (7)
C48—C47—H47	120.2	F72—P7—F72^{ii}	180.0 (10)
C46—C47—H47	120.2	F73^{ii}—P7—F71^{ii}	87.9 (6)
C47—C48—C49	120.4 (8)	F73—P7—F71^{ii}	92.1 (6)
C47—C48—H48	119.8	F72—P7—F71^{ii}	93.3 (5)
C49—C48—H48	119.8	F72^{ii}—P7—F71^{ii}	86.7 (5)
C48—C49—C50	118.8 (8)	F73^{ii}—P7—F71	92.1 (6)
C48—C49—H49	120.6	F73—P7—F71	87.9 (6)
C50—C49—H49	120.6	F72—P7—F71	86.7 (5)
N12—C50—C49	120.2 (7)	F72^{ii}—P7—F71	93.3 (5)
N12—C50—C51	114.5 (5)	F71^{ii}—P7—F71	180.0 (10)
C49—C50—C51	125.3 (7)	N2—Pd1—O1	176.5 (2)
N13—C51—C52	118.7 (6)	N2—Pd1—N3	80.9 (2)
N13—C51—C50	113.3 (5)	O1—Pd1—N3	98.5 (2)
C52—C51—C50	128.0 (6)	N2—Pd1—N1	80.5 (2)
C53—C52—C51	119.2 (7)	O1—Pd1—N1	100.3 (2)
C53—C52—H52	120.4	N3—Pd1—N1	160.9 (2)
C51—C52—H52	120.4	N2—Pd1—Pd2	100.70 (16)
C52—C53—C54	121.0 (7)	O1—Pd1—Pd2	76.11 (15)
C52—C53—H53	119.5	N3—Pd1—Pd2	106.22 (17)
C54—C53—H53	119.5	N1—Pd1—Pd2	81.66 (15)
C53—C54—C55	119.0 (8)	N6—Pd2—O3	179.5 (2)
C53—C54—H54	120.5	N6—Pd2—N7	81.2 (2)
C55—C54—H54	120.5	O3—Pd2—N7	98.98 (19)
N13—C55—C54	118.8 (6)	N6—Pd2—N5	81.1 (2)
N13—C55—C56	112.9 (5)	O3—Pd2—N5	98.8 (2)
C54—C55—C56	128.2 (6)	N7—Pd2—N5	162.1 (2)
N14—C56—C57	121.7 (6)	N6—Pd2—Pd1	98.75 (15)
N14—C56—C55	114.2 (5)	O3—Pd2—Pd1	80.84 (12)
C57—C56—C55	124.0 (6)	N7—Pd2—Pd1	81.19 (15)
C58—C57—C56	117.8 (7)	N5—Pd2—Pd1	103.92 (15)
C58—C57—H57	121.1	N9—Pd3—O5	175.6 (2)
C56—C57—H57	121.1	N9—Pd3—N10	80.8 (2)
C57—C58—C59	120.7 (7)	O5—Pd3—N10	98.7 (2)

C57—C58—H58	119.7	N9—Pd3—N8	80.8 (3)
C59—C58—H58	119.7	O5—Pd3—N8	100.0 (3)
C60—C59—C58	117.8 (7)	N10—Pd3—N8	160.8 (2)
C60—C59—H59	121.1	N9—Pd3—Pd4	99.25 (16)
C58—C59—H59	121.1	O5—Pd3—Pd4	76.68 (17)
N14—C60—C59	122.8 (7)	N10—Pd3—Pd4	107.76 (16)
N14—C60—H60	118.6	N8—Pd3—Pd4	80.80 (15)
C59—C60—H60	118.6	N13—Pd4—O4	179.0 (2)
N15—C61—C62	178 (2)	N13—Pd4—N14	81.1 (2)
C61—C62—H62A	110.0	O4—Pd4—N14	99.6 (2)
C61—C62—H62B	109.3	N13—Pd4—N12	81.0 (2)
H62A—C62—H62B	109.4	O4—Pd4—N12	98.3 (2)
C61—C62—H62C	109.3	N14—Pd4—N12	161.9 (2)
H62A—C62—H62C	109.4	N13—Pd4—Pd3	100.39 (15)
H62B—C62—H62C	109.4	O4—Pd4—Pd3	80.48 (14)
C1—N1—C5	119.3 (6)	N14—Pd4—Pd3	81.66 (15)
C1—N1—Pd1	127.5 (5)	N12—Pd4—Pd3	103.64 (14)

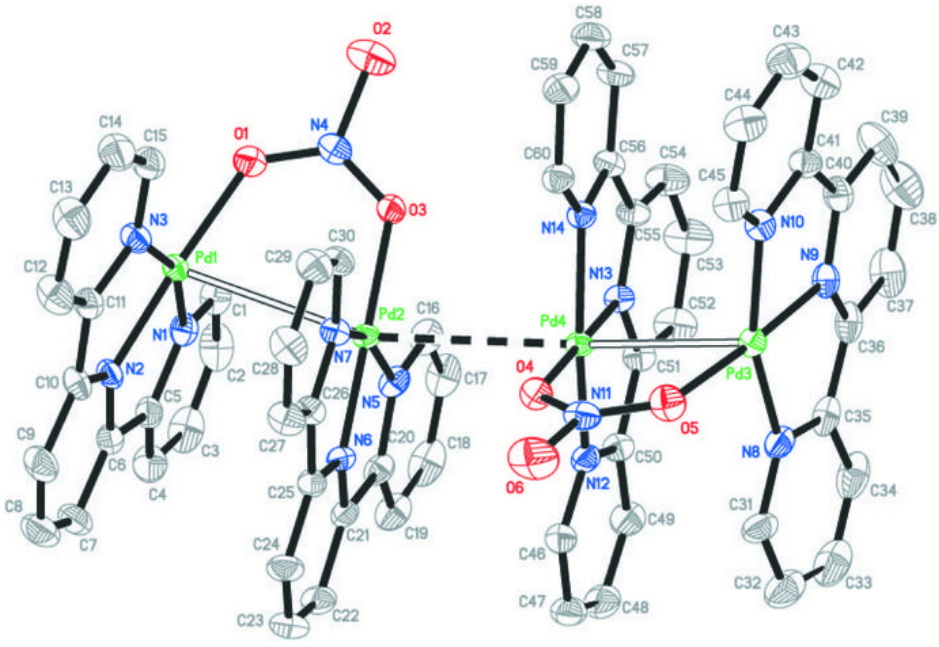
Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*+2, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···F33	0.93	2.52	3.313 (12)	144
C3—H3···F13^{iii}	0.93	2.47	3.402 (12)	176
C7—H7···F44^{iv}	0.93	2.45	3.223 (13)	140
C14—H14···F13	0.93	2.54	3.246 (11)	133
C16—H16···F33	0.93	2.32	3.051 (11)	135
C17—H17···F34^{v}	0.93	2.46	3.291 (11)	150
C18—H18···F12^{iii}	0.93	2.52	3.251 (12)	135
C22—H22···F43^{iv}	0.93	2.45	3.104 (11)	127
C24—H24···F52^{vi}	0.93	2.49	3.367 (9)	157
C30—H30···F15	0.93	2.39	3.192 (9)	145
C34—H34···N15^{iii}	0.93	2.47	3.157 (16)	131
C38—H38···F71^{vii}	0.93	2.33	3.159 (12)	148
C39—H39···F62^{viii}	0.93	2.54	3.474 (13)	179
C48—H48···F54^{iii}	0.93	2.42	3.129 (11)	133
C52—H52···F31^{v}	0.93	2.46	3.254 (11)	143
C54—H54···F11^{viii}	0.93	2.39	3.304 (10)	166
C60—H60···F51	0.93	2.34	3.188 (9)	151

Symmetry codes: (iii) *x*+1, *y*, *z*; (iv) −*x*+2, −*y*+1, −*z*+1; (v) −*x*+2, −*y*+1, −*z*; (vi) −*x*+1, −*y*+1, −*z*+1; (vii) *x*, *y*+1, *z*; (viii) −*x*+1, −*y*+1, −*z*.

Fig. 1


O2
O1
N4
O3
C14
C15
C13
N3
Pd1
C12
C11
C30
C29
C1
N1
Pd2
C16
C10
N2
C28
N7
C17
C2
C5
C26
N5
C9
C6
C27
N6
C20
C18
C3
C4
C25
C21
C19
C8
C7
C24
C23
C22
C58
C57
C59
C43
C42
C44
C39
C60
C56
C54
C41
C40
C45
C38
N14
C55
N10
C53
N13
N9
C37
C52
Pd4
C36
O4
C51
Pd3
N11
O5
C35
C50
N8
O6
N12
C34
C49
C31
C46
C33
C47
C48
C32