IUCrData

ISSN 2414-3146

(2,2′-Bipyridine-κ^2N,N')(4,4′-dimethoxy-2,2′-bipyridine-κ^2N,N')palladium(II) bis(trifluoromethanesulfonate)

Brittney B. Vargas,[a] Hadi D. Arman[b] and Rafael A. Adrian[a]*

[a]Department of Chemistry and Biochemistry, University of the Incarnate Word, San Antonio, Texas 78209, USA, and [b]Department of Chemistry, The University of Texas at San Antonio, San Antonio, Texas 78249, USA. *Correspondence e-mail: adrian@uiwtx.edu

Received 16 January 2024
Accepted 31 January 2024

Edited by M. Weil, Vienna University of Technology, Austria

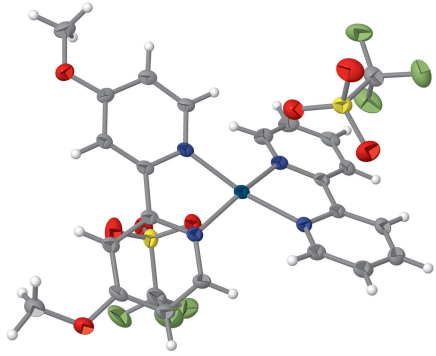
Keywords: crystal structure; palladium(II) complex; square-planar coordination environment; 2,2′-bipyridine; 4,4′-dimethoxy-2,2′-bipyridine; trifluoromethanesulfonate salt; τ_4 descriptor.

CCDC reference: 2330055

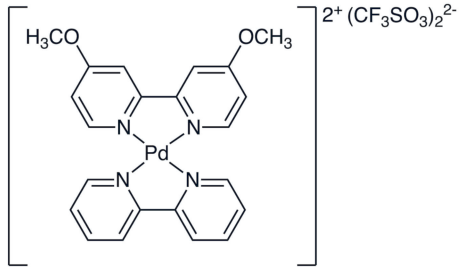
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex salt, $[Pd(C_{10}H_8N_2)(C_{12}H_{12}N_2O_2)](CF_3SO_3)_2$, the palladium(II) atom is fourfold coordinated by two chelating ligands, 2,2′-bipyridine and 4,4′-dimethoxy-2,2′-bipyridine, in a distorted square-planar environment. In the crystal, weak π–π stacking interactions between the 2,2′-bipyridine rings [centroid-to-centroid distances = 3.8984 (19) Å] and between the 4,4′-dimethoxy-2,2′-bipyridine rings [centroid-to-centroid distances = 3.747 (18) Å] contribute to the alignment of the complex cations in columns parallel to the *b*-axis direction.

3D view



Chemical scheme



Structure description

Bipyridine derivatives continue to be recognized as valuable ligands for the synthesis of new transition-metal complexes, including cobalt(II) (Kondori *et al.*, 2021), ruthenium(II) (Benson *et al.*, 2021; Maier *et al.*, 2022), iron(II) (Karges & Gasser, 2020), copper(II) (Shchegolkov *et al.*, 2021) and palladium(II) (Komlyagina *et al.*, 2023) to mention a few. Recently, palladium(II) complexes containing 2,2′-bipyridine as ligand have shown significant cytotoxicity against HT-29 (colorectal adenocarcinoma), MCF-7 (breast), and HeLa (human squamous cervical adenocarcinoma) cancer cell lines (Tabrizi *et al.*, 2020). As part of our research in this area, we describe herein the synthesis and structure of the title palladium(II) complex.

The asymmetric unit comprises one complex cation and two trifluoromethanesulfonate anions. The palladium(II) atom shows a distorted square-planar coordination environment defined by a bidentate 2,2′-bipyridine ligand and a bidentate 4,4′-dimethoxy-2,2′-bipyridine; trifluoromethanesulfonate ions sit in the outer coordination sphere, balancing the charge of the complex metal cation (Fig. 1). The Pd—N bond lengths are in good agreement with those in comparable square-planar 4,4′-dimethoxy-2,2′-bipyridine

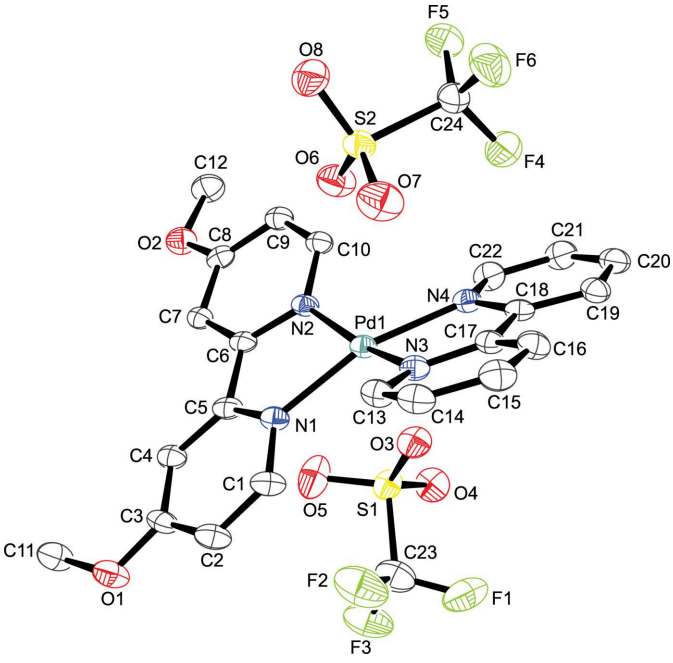


Figure 1
The structures of the molecular entities present in title compound with displacement ellipsoids drawn at the 50% probability level; H atoms are omitted for clarity.

palladium(II) complexes currently available in the Cambridge Structural Database (CSD, version 5.45, Nov 2023; Groom *et al.*, 2016): refcodes BEPVIF (Yang *et al.*, 2022), WISQUO (Komlyagina *et al.*, 2023); WISRAV (Komlyagina *et al.*, 2023). The τ_4 descriptor value (Yang *et al.*, 2007) of 0.22 reflects a significant distortion from a perfect square-planar coordination ($\tau_4 = 0$). Numerical data for relevant bond lengths and angles are presented in Table 1.

In the extended structure, the complex packs into columns extending parallel to the *b* axis (Fig. 2). Contiguous pyridine rings show weak π–π stacking interactions, with centroid-to-centroid distances ($Cg\cdots Cg$) alternating between 3.7472 (18) Å (between 4,4′-dimethoxy-2,2′-bipyridine ligands) and 3.8984 (19) Å (between 2,2′-bipyridine ligands), and offset distances of 1.641 and 1.769 Å, respectively (Fig. 3). No other significant supramolecular interactions are present in the crystal packing of the title compound.

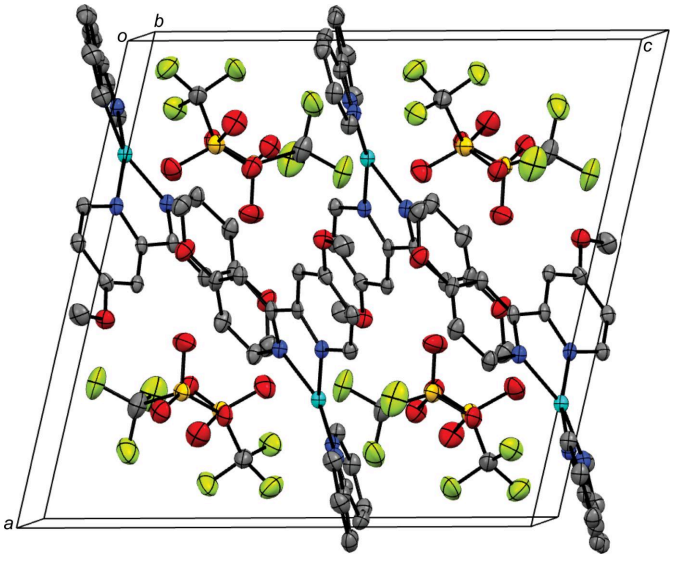


Figure 2
Perspective view of the crystal packing of the title complex approximately along the *b* axis; H atoms are omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Pd1—N2	2.022 (3)	Pd1—N3	2.033 (3)
Pd1—N1	2.029 (3)	Pd1—N4	2.046 (3)
N2—Pd1—N1	79.63 (10)	N2—Pd1—N4	101.76 (10)
N2—Pd1—N3	165.80 (10)	N1—Pd1—N4	162.05 (10)
N1—Pd1—N3	102.93 (10)	N3—Pd1—N4	80.18 (10)

Synthesis and crystallization

The title complex was prepared by adding $Ag(CF_3SO_3)$ (0.0771 g, 0.300 mmol) to an acetonitrile suspension (40 ml) of [Pd(2,2′-bipyridine)Cl_2] (0.100 g, 0.300 mmol). The mixture was heated, with stirring, at 333 K for 2 h and then filtered using a PTFE syringe filter to remove the precipitated AgCl. 4,4′-Dimethoxy-2,2′-bipyridine (0.0649 g, 0.300 mmol) was added to the resulting solution and heated at 343 K to reduce the volume of the solution to 10 ml. X-ray diffraction quality crystals of the title complex were obtained by vapor diffusion of ether over the resulting concentrated acetonitrile solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We are thankful for the support of the Department of Chemistry and Biochemistry at the University of the Incarnate Word and the X-ray Diffraction Laboratory at the University of Texas at San Antonio.

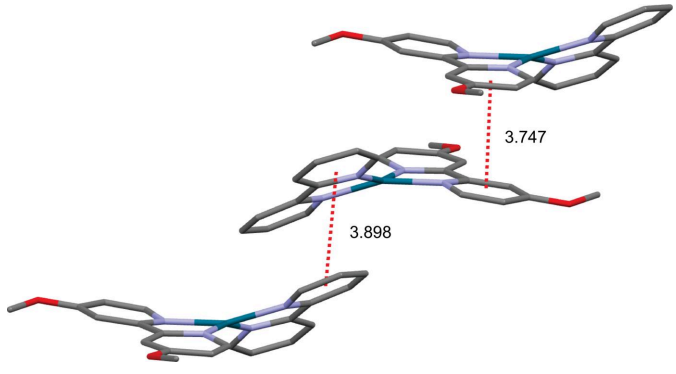


Figure 3
Capped sticks representation of the complex cation showing π–π stacking interactions (red). H atoms and anions are omitted for clarity.

Funding information

Funding for this research was provided by: National Science Foundation (award No. 1920059); Welch Foundation (award No. BN0032); University of the Incarnate Word Faculty Endowed Research Award; Constance and Miriam Jauchler Jones Endowed Chair.

References

Benson, K. R., Stash, J., Moffa, K. L., Schmehl, R. H., Dudley, T. J. & Paul, J. J. (2021). *Polyhedron*, **205**, 115300.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Karges, J. & Gasser, G. (2020). *Inorg. Chim. Acta*, **499**, 119196.
Komlyagina, V. I., Romashev, N. F., Besprozvannykh, V. K., Arakelyan, J., Wu, C., Chubarov, A. S., Bakaev, I. V., Soh, Y. K., Abramov, P. A., Cheung, K. L., Kompan'kov, N. B., Ryadun, A. A., Babak, M. V. & Gushchin, A. L. (2023). *Inorg. Chem.* **62**, 11541–11553.
Kondori, T., Shahraki, O., Akbarzadeh-T, N. & Aramesh-Boroujeni, Z. (2021). *J. Biomol. Struct. Dyn.* **39**, 595–609.
Maier, A. S., Thomas, C., Kränzlein, M., Pehl, T. M. & Rieger, B. (2022). *Macromolecules*, **55**, 7039–7048.
Rigaku OD (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction. Yarnton, England.
Shchegolkov, E. V., Shchur, I. V., Burgart, Y. V., Slepukhin, P. A., Evstigneeva, N. P., Gerasimova, N. A., Zilberberg, N. V., Kungurov, N. V., Saloutin, V. I. & Chupakhin, O. N. (2021). *Polyhedron*, **194**, 114900.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Tabrizi, L., Zouchoune, B. & Zaiter, A. (2020). *Inorg. Chim. Acta*, **499**, 119211.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pd(C_{10}H_8N_2)(C_{12}H_{12}N_2O_2)](CF_3SO_3)_2$
M_r	776.96
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	14.4340 (3), 13.9644 (2), 14.2126 (2)
β (°)	102.5361 (16)
V (Å^3)	2796.41 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	7.64
Crystal size (mm)	0.23 × 0.11 × 0.08
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.512, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26480, 5585, 5101
R_{int}	0.053
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.100, 1.04
No. of reflections	5585
No. of parameters	408
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.80, −1.09

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), and *OLEX2* (Dolomanov *et al.*, 2009).

Yang, G., Wu, H., Gallarati, S., Corminboeuf, C., Wang, Q. & Zhu, J. (2022). *J. Am. Chem. Soc.* **144**, 14047–14052.
Yang, L., Powell, D. R. & Houser, R. P. (2007). *Dalton Trans.* pp. 955–964.

full crystallographic data

IUCrData (2024). **9**, x240109 [https://doi.org/10.1107/S2414314624001093]

(2,2′-Bipyridine-κ^2N,N')(4,4′-dimethoxy-2,2′-bipyridine-κ^2N,N')palladium(II) bis(trifluoromethanesulfonate)

Brittney B. Vargas, Hadi D. Arman and Rafael A. Adrian

(2,2′-Bipyridine-κ^2N,N')(4,4′-dimethoxy-2,2′-bipyridine-κ^2N,N')palladium(II) bis(trifluoromethanesulfonate)

Crystal data

$[Pd(C_{10}H_8N_2)(C_{12}H_{12}N_2O_2)](CF_3SO_3)_2$
M_r = 776.96
Monoclinic, $P2_1/c$
a = 14.4340 (3) Å
b = 13.9644 (2) Å
c = 14.2126 (2) Å
β = 102.5361 (16)°
V = 2796.41 (8) Å^3
Z = 4
$F(000)$ = 1552
D_x = 1.845 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 13876 reflections
θ = 4.4–75.4°
μ = 7.64 mm^{-1}
T = 100 K
Block, yellow
0.23 × 0.11 × 0.08 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.512, T_{max} = 1.000
26480 measured reflections
5585 independent reflections
5101 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 76.2°, θ_{min} = 3.1°
h = −17→18
k = −17→16
l = −15→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 1.04
5585 reflections
408 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 5.4251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −1.09 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.25207 (2)	0.48236 (2)	0.49500 (2)	0.02008 (9)
S2	0.22124 (6)	0.40289 (6)	0.19795 (6)	0.02732 (18)
S1	0.27163 (6)	0.63092 (6)	0.75710 (6)	0.02833 (18)
F5	0.15001 (17)	0.55231 (18)	0.09497 (18)	0.0472 (6)
O2	0.58599 (17)	0.76062 (17)	0.54340 (17)	0.0310 (5)
O3	0.22186 (18)	0.59380 (19)	0.66506 (17)	0.0351 (6)
F6	0.06435 (18)	0.4276 (2)	0.06797 (18)	0.0533 (6)
F4	0.06969 (19)	0.5071 (2)	0.19721 (18)	0.0548 (7)
O6	0.2702 (2)	0.4622 (2)	0.27515 (19)	0.0406 (6)
F1	0.1486 (2)	0.5453 (2)	0.84015 (18)	0.0586 (7)
O1	0.55650 (19)	0.32506 (19)	0.82842 (18)	0.0365 (6)
F3	0.2887 (2)	0.5636 (2)	0.93124 (17)	0.0641 (8)
O7	0.1755 (2)	0.3204 (2)	0.2284 (2)	0.0481 (7)
O5	0.37298 (19)	0.6267 (2)	0.7740 (2)	0.0495 (8)
N1	0.35491 (19)	0.41902 (19)	0.59584 (18)	0.0224 (5)
N3	0.15739 (19)	0.37451 (19)	0.45377 (18)	0.0222 (5)
O8	0.2716 (2)	0.3841 (2)	0.1230 (2)	0.0430 (7)
O4	0.2332 (2)	0.71853 (19)	0.78532 (19)	0.0389 (6)
F2	0.2640 (3)	0.4555 (2)	0.8203 (2)	0.0700 (9)
N4	0.13534 (19)	0.56042 (19)	0.43114 (18)	0.0229 (5)
N2	0.35692 (19)	0.58047 (18)	0.50606 (17)	0.0212 (5)
C5	0.4350 (2)	0.4719 (2)	0.6269 (2)	0.0220 (6)
C17	0.0694 (2)	0.4035 (2)	0.4067 (2)	0.0222 (6)
C1	0.3429 (3)	0.3403 (2)	0.6465 (2)	0.0285 (7)
H1	0.285816	0.304663	0.627345	0.034*
C13	0.1788 (2)	0.2810 (2)	0.4545 (2)	0.0259 (7)
H13	0.241428	0.261207	0.483592	0.031*
C8	0.5106 (2)	0.7026 (2)	0.5260 (2)	0.0225 (6)
C19	−0.0320 (2)	0.5509 (2)	0.3674 (2)	0.0256 (7)
H19	−0.087525	0.513068	0.347393	0.031*
C4	0.5058 (2)	0.4444 (2)	0.7039 (2)	0.0237 (6)
H4	0.561670	0.481893	0.722918	0.028*
C6	0.4383 (2)	0.5611 (2)	0.5720 (2)	0.0204 (6)
C9	0.4295 (2)	0.7186 (2)	0.4548 (2)	0.0244 (6)
H9	0.425302	0.772082	0.412835	0.029*
C10	0.3557 (2)	0.6550 (2)	0.4466 (2)	0.0227 (6)
H10	0.301173	0.664352	0.396410	0.027*
C22	0.1284 (3)	0.6560 (2)	0.4315 (2)	0.0293 (7)
H22	0.183625	0.692736	0.456607	0.035*
C14	0.1131 (3)	0.2125 (2)	0.4144 (2)	0.0296 (7)
H14	0.130078	0.146652	0.416703	0.036*
C15	0.0224 (3)	0.2410 (3)	0.3710 (2)	0.0307 (7)
H15	−0.024666	0.194961	0.345058	0.037*
C18	0.0555 (2)	0.5074 (2)	0.4013 (2)	0.0230 (6)
C3	0.4941 (3)	0.3607 (2)	0.7530 (2)	0.0268 (7)

C16	0.0009 (2)	0.3377 (3)	0.3657 (2)	0.0283 (7)
H16	−0.060524	0.358768	0.334111	0.034*
C20	−0.0376 (3)	0.6500 (3)	0.3631 (2)	0.0302 (7)
H20	−0.096400	0.680803	0.337457	0.036*
C7	0.5165 (2)	0.6199 (2)	0.5829 (2)	0.0201 (6)
H7	0.573299	0.604693	0.628131	0.024*
C2	0.4095 (3)	0.3096 (2)	0.7245 (2)	0.0303 (7)
H2	0.398274	0.253950	0.758903	0.036*
C24	0.1222 (3)	0.4770 (3)	0.1370 (3)	0.0334 (8)
C21	0.0431 (3)	0.7033 (3)	0.3965 (3)	0.0322 (7)
H21	0.040546	0.771242	0.395580	0.039*
C12	0.5745 (3)	0.8532 (3)	0.4959 (3)	0.0364 (8)
H12A	0.556581	0.844023	0.425981	0.055*
H12B	0.634444	0.888665	0.512401	0.055*
H12C	0.524744	0.889479	0.517390	0.055*
C11	0.6492 (3)	0.3687 (3)	0.8529 (3)	0.0374 (8)
H11A	0.677878	0.368095	0.796451	0.056*
H11B	0.689463	0.332793	0.905511	0.056*
H11C	0.643101	0.435020	0.873438	0.056*
C23	0.2422 (3)	0.5447 (3)	0.8415 (3)	0.0438 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.02596 (14)	0.01770 (14)	0.01692 (13)	0.00027 (8)	0.00541 (9)	−0.00010 (8)
S2	0.0326 (4)	0.0236 (4)	0.0260 (4)	0.0005 (3)	0.0068 (3)	0.0021 (3)
S1	0.0303 (4)	0.0315 (4)	0.0237 (4)	−0.0033 (3)	0.0070 (3)	−0.0117 (3)
F5	0.0499 (13)	0.0452 (14)	0.0478 (13)	0.0092 (11)	0.0134 (11)	0.0216 (11)
O2	0.0348 (13)	0.0276 (12)	0.0310 (12)	−0.0050 (10)	0.0080 (10)	0.0008 (10)
O3	0.0414 (14)	0.0410 (14)	0.0232 (11)	−0.0027 (11)	0.0075 (10)	−0.0128 (10)
F6	0.0484 (14)	0.0636 (17)	0.0412 (13)	0.0002 (12)	−0.0051 (10)	−0.0074 (12)
F4	0.0526 (15)	0.0778 (18)	0.0388 (13)	0.0264 (13)	0.0206 (11)	0.0045 (12)
O6	0.0447 (15)	0.0442 (15)	0.0308 (13)	−0.0057 (12)	0.0033 (11)	0.0030 (12)
F1	0.0636 (17)	0.0736 (18)	0.0437 (14)	−0.0250 (14)	0.0230 (12)	−0.0032 (13)
O1	0.0430 (14)	0.0343 (14)	0.0292 (12)	−0.0049 (11)	0.0012 (11)	0.0096 (11)
F3	0.093 (2)	0.0685 (19)	0.0246 (11)	−0.0018 (16)	−0.0006 (12)	−0.0001 (12)
O7	0.0592 (18)	0.0342 (15)	0.0493 (16)	−0.0108 (13)	0.0081 (14)	0.0058 (13)
O5	0.0331 (14)	0.067 (2)	0.0491 (16)	−0.0068 (13)	0.0096 (12)	−0.0278 (15)
N1	0.0283 (13)	0.0210 (13)	0.0178 (12)	−0.0009 (10)	0.0050 (10)	0.0000 (10)
N3	0.0279 (13)	0.0211 (13)	0.0176 (12)	−0.0021 (10)	0.0050 (10)	−0.0019 (10)
O8	0.0493 (16)	0.0425 (16)	0.0413 (15)	0.0132 (13)	0.0187 (12)	0.0002 (12)
O4	0.0479 (15)	0.0321 (13)	0.0366 (14)	0.0009 (12)	0.0088 (12)	−0.0113 (11)
F2	0.111 (3)	0.0356 (14)	0.0587 (17)	0.0080 (15)	0.0078 (17)	0.0039 (13)
N4	0.0291 (13)	0.0217 (13)	0.0193 (12)	0.0016 (11)	0.0082 (10)	0.0010 (10)
N2	0.0288 (13)	0.0197 (12)	0.0157 (11)	0.0025 (10)	0.0062 (10)	−0.0002 (10)
C5	0.0340 (17)	0.0185 (15)	0.0151 (13)	0.0003 (12)	0.0085 (12)	−0.0030 (11)
C17	0.0281 (15)	0.0228 (15)	0.0160 (13)	0.0010 (12)	0.0058 (11)	0.0000 (11)
C1	0.0384 (18)	0.0258 (17)	0.0212 (15)	−0.0060 (14)	0.0059 (13)	0.0032 (13)

C13	0.0351 (17)	0.0197 (15)	0.0229 (15)	0.0018 (13)	0.0064 (13)	0.0001 (12)
C8	0.0302 (16)	0.0176 (14)	0.0223 (14)	−0.0023 (12)	0.0116 (12)	−0.0036 (12)
C19	0.0298 (16)	0.0282 (17)	0.0185 (14)	0.0019 (13)	0.0044 (12)	0.0004 (12)
C4	0.0317 (16)	0.0221 (16)	0.0176 (13)	0.0005 (13)	0.0062 (12)	−0.0020 (12)
C6	0.0310 (16)	0.0178 (15)	0.0138 (13)	0.0037 (12)	0.0084 (11)	−0.0024 (11)
C9	0.0338 (17)	0.0200 (15)	0.0211 (14)	0.0035 (13)	0.0099 (12)	0.0001 (12)
C10	0.0287 (16)	0.0204 (15)	0.0197 (14)	0.0022 (12)	0.0069 (12)	0.0027 (12)
C22	0.0372 (18)	0.0207 (16)	0.0321 (17)	0.0019 (13)	0.0120 (14)	−0.0003 (13)
C14	0.0432 (19)	0.0212 (16)	0.0246 (16)	−0.0003 (14)	0.0078 (14)	−0.0006 (13)
C15	0.0383 (18)	0.0289 (18)	0.0245 (16)	−0.0066 (14)	0.0058 (14)	−0.0040 (14)
C18	0.0296 (16)	0.0261 (16)	0.0139 (13)	−0.0006 (13)	0.0055 (12)	0.0008 (11)
C3	0.0370 (17)	0.0268 (17)	0.0153 (13)	0.0049 (14)	0.0028 (12)	0.0029 (12)
C16	0.0319 (17)	0.0310 (17)	0.0204 (14)	−0.0015 (14)	0.0018 (12)	−0.0003 (13)
C20	0.0378 (18)	0.0318 (18)	0.0224 (15)	0.0098 (14)	0.0095 (13)	0.0049 (13)
C7	0.0271 (15)	0.0184 (14)	0.0152 (13)	0.0030 (12)	0.0056 (11)	−0.0028 (11)
C2	0.0430 (19)	0.0228 (16)	0.0240 (15)	−0.0051 (14)	0.0047 (14)	0.0049 (13)
C24	0.0339 (18)	0.040 (2)	0.0260 (17)	0.0054 (15)	0.0059 (14)	−0.0004 (15)
C21	0.041 (2)	0.0244 (17)	0.0346 (18)	0.0065 (14)	0.0156 (15)	0.0030 (14)
C12	0.044 (2)	0.0284 (19)	0.0395 (19)	−0.0049 (15)	0.0140 (16)	0.0058 (15)
C11	0.043 (2)	0.037 (2)	0.0296 (18)	−0.0039 (16)	0.0015 (15)	0.0068 (15)
C23	0.061 (3)	0.039 (2)	0.0279 (18)	0.0000 (19)	0.0018 (17)	−0.0034 (16)

Geometric parameters (Å, º)

Pd1—N2	2.022 (3)	C1—C2	1.370 (5)
Pd1—N1	2.029 (3)	C1—H1	0.9500
Pd1—N3	2.033 (3)	C13—C14	1.380 (5)
Pd1—N4	2.046 (3)	C13—H13	0.9500
S2—O6	1.433 (3)	C8—C9	1.389 (5)
S2—O8	1.438 (3)	C8—C7	1.402 (4)
S2—O7	1.440 (3)	C19—C20	1.388 (5)
S2—C24	1.824 (4)	C19—C18	1.391 (5)
S1—O5	1.431 (3)	C19—H19	0.9500
S1—O4	1.436 (3)	C4—C3	1.390 (5)
S1—O3	1.445 (2)	C4—H4	0.9500
S1—C23	1.814 (4)	C6—C7	1.377 (4)
F5—C24	1.314 (5)	C9—C10	1.372 (5)
O2—C8	1.336 (4)	C9—H9	0.9500
O2—C12	1.451 (4)	C10—H10	0.9500
F6—C24	1.335 (4)	C22—C21	1.391 (5)
F4—C24	1.328 (4)	C22—H22	0.9500
F1—C23	1.347 (5)	C14—C15	1.380 (5)
O1—C3	1.338 (4)	C14—H14	0.9500
O1—C11	1.442 (5)	C15—C16	1.383 (5)
F3—C23	1.333 (4)	C15—H15	0.9500
N1—C1	1.345 (4)	C3—C2	1.396 (5)
N1—C5	1.362 (4)	C16—H16	0.9500
N3—C13	1.342 (4)	C20—C21	1.376 (5)

N3—C17	1.362 (4)	C20—H20	0.9500
F2—C23	1.335 (5)	C7—H7	0.9500
N4—C22	1.338 (4)	C2—H2	0.9500
N4—C18	1.358 (4)	C21—H21	0.9500
N2—C10	1.338 (4)	C12—H12A	0.9800
N2—C6	1.361 (4)	C12—H12B	0.9800
C5—C4	1.380 (4)	C12—H12C	0.9800
C5—C6	1.476 (4)	C11—H11A	0.9800
C17—C16	1.382 (5)	C11—H11B	0.9800
C17—C18	1.465 (4)	C11—H11C	0.9800

N2—Pd1—N1	79.63 (10)	C8—C9—H9	120.9
N2—Pd1—N3	165.80 (10)	N2—C10—C9	123.1 (3)
N1—Pd1—N3	102.93 (10)	N2—C10—H10	118.4
N2—Pd1—N4	101.76 (10)	C9—C10—H10	118.4
N1—Pd1—N4	162.05 (10)	N4—C22—C21	122.2 (3)
N3—Pd1—N4	80.18 (10)	N4—C22—H22	118.9
O6—S2—O8	115.34 (18)	C21—C22—H22	118.9
O6—S2—O7	114.46 (17)	C15—C14—C13	119.0 (3)
O8—S2—O7	114.52 (18)	C15—C14—H14	120.5
O6—S2—C24	103.93 (17)	C13—C14—H14	120.5
O8—S2—C24	102.87 (17)	C14—C15—C16	119.1 (3)
O7—S2—C24	103.50 (18)	C14—C15—H15	120.5
O5—S1—O4	115.52 (17)	C16—C15—H15	120.5
O5—S1—O3	115.24 (16)	N4—C18—C19	121.0 (3)
O4—S1—O3	114.33 (16)	N4—C18—C17	115.2 (3)
O5—S1—C23	103.9 (2)	C19—C18—C17	123.7 (3)
O4—S1—C23	102.74 (18)	O1—C3—C4	125.5 (3)
O3—S1—C23	102.63 (17)	O1—C3—C2	115.9 (3)
C8—O2—C12	116.6 (3)	C4—C3—C2	118.6 (3)
C3—O1—C11	117.7 (3)	C17—C16—C15	119.6 (3)
C1—N1—C5	118.0 (3)	C17—C16—H16	120.2
C1—N1—Pd1	125.0 (2)	C15—C16—H16	120.2
C5—N1—Pd1	115.6 (2)	C21—C20—C19	119.1 (3)
C13—N3—C17	118.8 (3)	C21—C20—H20	120.4
C13—N3—Pd1	125.4 (2)	C19—C20—H20	120.4
C17—N3—Pd1	114.7 (2)	C6—C7—C8	118.8 (3)
C22—N4—C18	119.1 (3)	C6—C7—H7	120.6
C22—N4—Pd1	125.8 (2)	C8—C7—H7	120.6
C18—N4—Pd1	114.2 (2)	C1—C2—C3	119.4 (3)
C10—N2—C6	118.7 (3)	C1—C2—H2	120.3
C10—N2—Pd1	124.8 (2)	C3—C2—H2	120.3
C6—N2—Pd1	116.0 (2)	F5—C24—F4	108.3 (3)
N1—C5—C4	122.4 (3)	F5—C24—F6	106.5 (3)
N1—C5—C6	114.1 (3)	F4—C24—F6	106.5 (3)
C4—C5—C6	123.4 (3)	F5—C24—S2	112.6 (3)
N3—C17—C16	121.0 (3)	F4—C24—S2	111.8 (3)
N3—C17—C18	115.0 (3)	F6—C24—S2	110.8 (3)

C16—C17—C18	124.0 (3)	C20—C21—C22	119.0 (3)
N1—C1—C2	122.7 (3)	C20—C21—H21	120.5
N1—C1—H1	118.7	C22—C21—H21	120.5
C2—C1—H1	118.7	O2—C12—H12A	109.5
N3—C13—C14	122.4 (3)	O2—C12—H12B	109.5
N3—C13—H13	118.8	H12A—C12—H12B	109.5
C14—C13—H13	118.8	O2—C12—H12C	109.5
O2—C8—C9	124.1 (3)	H12A—C12—H12C	109.5
O2—C8—C7	116.7 (3)	H12B—C12—H12C	109.5
C9—C8—C7	119.2 (3)	O1—C11—H11A	109.5
C20—C19—C18	119.4 (3)	O1—C11—H11B	109.5
C20—C19—H19	120.3	H11A—C11—H11B	109.5
C18—C19—H19	120.3	O1—C11—H11C	109.5
C5—C4—C3	118.8 (3)	H11A—C11—H11C	109.5
C5—C4—H4	120.6	H11B—C11—H11C	109.5
C3—C4—H4	120.6	F3—C23—F2	107.8 (3)
N2—C6—C7	121.5 (3)	F3—C23—F1	107.9 (4)
N2—C6—C5	114.2 (3)	F2—C23—F1	106.7 (4)
C7—C6—C5	124.3 (3)	F3—C23—S1	111.1 (3)
C10—C9—C8	118.3 (3)	F2—C23—S1	111.7 (3)
C10—C9—H9	120.9	F1—C23—S1	111.4 (3)