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ISSN 2414-3146

Bis[*S*-hexyl 3-(thiophen-2-ylmethylidene)dithiocarbazato-κ^2N^3,S]palladium(II)

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Received 15 June 2016
Accepted 12 July 2016

Edited by C. Rizzoli, Universita degli Studi di Parma, Italy

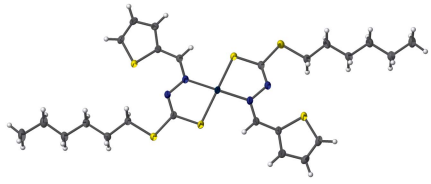
Keywords: crystal structure; palladium(II) complex; dithiocarbazate ligand.

CCDC reference: 1492179

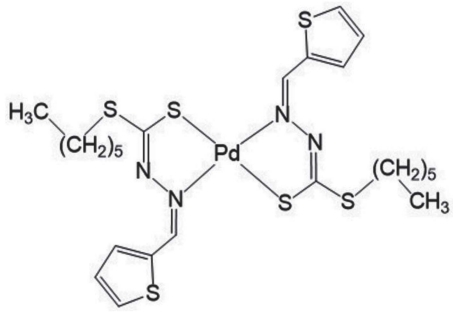
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[Pd(C_{12}H_{17}N_2S_3)_2]$, the Pd^{II} atom exhibits a square-planar coordination geometry with the *N*,*S*-chelating ligands arranged in a *trans* configuration. Intramolecular C—H···S hydrogen bonds are observed. In the crystal, molecules are linked by weak C—H···N hydrogen-bond interactions, forming chains parallel to the *b* axis.

3D view



Chemical scheme



Structure description

The title compound is isomorphous and isotypic to the bischelated copper(II) and nickel(II) complexes (Begum *et al.*, 2016). In the complex (Fig. 1), the two Schiff bases, in their deprotonated imino thiolate form, chelate the metal centre *via* the N1/N3 azomethine nitrogen and S2/S5 thiolate sulfur atoms in a *trans*-planar configuration exhibiting a pseudo-centrosymmetric arrangement. The molecular structure of similar non-coordinating ligands (Begum, Howlader *et al.*, 2015; Begum, Zangrando *et al.*, 2015) shows the *β*-nitrogen and the thioketo sulfur atoms are *trans* located with respect to the C6—N2 bond. Thus, upon coordination the deprotonated ligand requires rotation by 180° about this C—N bond in order to allow the *N*,*S* chelating behavior towards the metal. In the complex the ligand shows some geometrical variations with respect to the free species, the most significant being an elongation of the thioketo C6—S2 bond length with a concomitant decrease of the N1—C5 and increase of the N—N bond lengths. The molecular conformation is enforced by intramolecular C—H···S hydrogen bonds (Table 1). The hexyl chains exhibit all carbon atoms in an *anti* conformation, this conformation being recognized as an energy minimum. In the crystal (Fig. 2), molecules are arranged

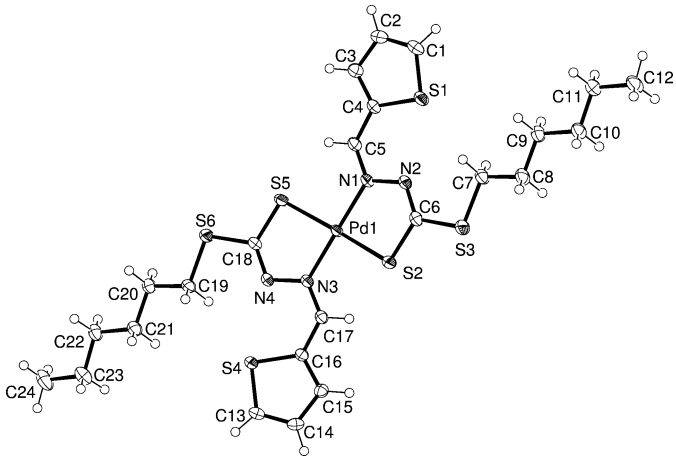


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

with the alkyl chains giving rise to a hydrophobic region and forming chains parallel to the *b* axis *via* weak C—H···N hydrogen bonds (Table 1).

Synthesis and crystallization

The title complex was prepared following a previously reported method (Begum *et al.*, 2016). A solution of $PdCl_2$ (0.044 g, 0.25 mmol) in 25 ml methanol was added to a solution of *S*-hexyl-3-(2-thienylidene)dithiocarbazate (0.144 g, 0.5 mmol) in 10 ml methanol. The resulting mixture was refluxed with constant stirring for 4 h. The orange–red precipitate formed was filtered off, washed with methanol and dried *in vacuo* over anhydrous $CaCl_2$. Orange–red single crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation from a mixture of dichloromethane and acetonitrile (3:1 *v*/*v*). M.p. = 352 K.

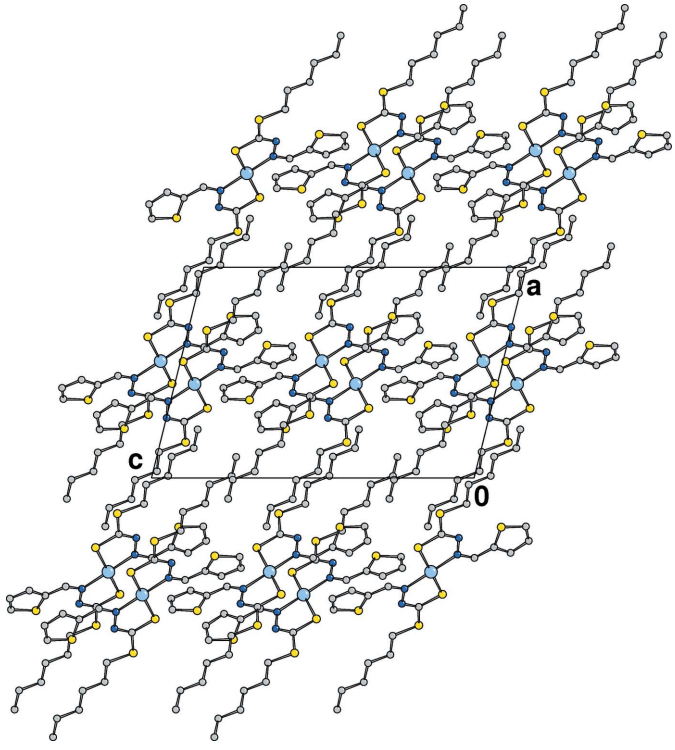


Figure 2
Crystal packing of the title complex viewed down the *b* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H4···S5	0.95	2.62	3.2970 (17)	129
C15—H20···N4^{i}	0.95	2.62	3.4088 (19)	141
C17—H21···S2	0.95	2.63	3.2596 (16)	124

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Pd(C_{12}H_{17}N_2S_3)_2]$
M_r	677.32
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	13.9118 (3), 10.37486 (19), 20.6696 (4)
β (°)	103.9290 (7)
V (Å^3)	2895.58 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.10
Crystal size (mm)	0.29 × 0.16 × 0.09
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.653, 0.906
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	27863, 6611, 5991
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.021, 0.055, 1.08
No. of reflections	6611
No. of parameters	318
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.41

Computer programs: *RAPID-AUTO* (Rigaku, 2010), *SIR92* (Altomare *et al.*, 1994), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Refinement

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

Acknowledgements

MSB is grateful to the Department of Chemistry, Rajshahi University, for the provision of laboratory facilities. MCS acknowledges the Department of Applied Chemistry, Toyama

University, for providing funds for single-crystal X-ray analyses.

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full crystallographic data

IUCrData (2016). **1**, x161132 [https://doi.org/10.1107/S2414314616011329]

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Bis[*S*-hexyl 3-(thiophen-2-ylmethylidene)dithiocarbazato-κ^2N^3,S]palladium(II)

Crystal data

$[Pd(C_{12}H_{17}N_2S_3)_2]$
M_r = 677.32
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.9118 (3) Å
b = 10.37486 (19) Å
c = 20.6696 (4) Å
β = 103.9290 (7)°
V = 2895.58 (10) Å^3
Z = 4
$F(000)$ = 1392.00
D_x = 1.554 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 23915 reflections
θ = 3.0–27.5°
μ = 1.10 mm^{-1}
T = 173 K
Prism, orange
0.29 × 0.16 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.653, T_{max} = 0.906
27863 measured reflections
6611 independent reflections
5991 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.026
θ_{max} = 27.5°
h = −18→16
k = −13→13
l = −26→26

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.055
S = 1.08
6611 reflections
318 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
$w = 1/[\sigma^2(F_o^2) + (0.030P)^2 + 0.7505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.445690 (8)	0.127519 (11)	0.438647 (5)	0.01874 (4)
S1	0.23361 (3)	0.07069 (4)	0.62208 (2)	0.02695 (9)
S2	0.33076 (3)	−0.01477 (4)	0.380204 (19)	0.02739 (9)
S3	0.16917 (3)	−0.14420 (4)	0.42171 (2)	0.03236 (10)
S4	0.62982 (3)	0.20479 (4)	0.243916 (18)	0.02268 (8)
S5	0.55236 (3)	0.28483 (4)	0.491361 (18)	0.02711 (9)
S6	0.69939 (3)	0.43033 (4)	0.44191 (2)	0.02856 (9)
N1	0.36382 (9)	0.11220 (12)	0.50727 (6)	0.0212 (3)
N2	0.28481 (9)	0.02514 (13)	0.49893 (6)	0.0230 (3)
N3	0.52642 (9)	0.14181 (12)	0.36967 (6)	0.0199 (3)
N4	0.59676 (9)	0.23996 (12)	0.37280 (6)	0.0210 (3)
C1	0.23047 (13)	0.13519 (17)	0.69779 (8)	0.0299 (4)
C2	0.29897 (12)	0.22996 (17)	0.71778 (8)	0.0291 (4)
C3	0.35536 (11)	0.25145 (16)	0.67058 (8)	0.0257 (3)
C4	0.32909 (11)	0.17267 (15)	0.61530 (7)	0.0215 (3)
C5	0.37951 (11)	0.17795 (15)	0.56243 (7)	0.0229 (3)
C6	0.26694 (11)	−0.03421 (15)	0.44212 (8)	0.0236 (3)
C7	0.12317 (12)	−0.14223 (16)	0.49665 (8)	0.0282 (4)
C8	0.03196 (12)	−0.22856 (17)	0.48830 (8)	0.0308 (4)
C9	−0.00963 (12)	−0.22185 (16)	0.54994 (8)	0.0289 (4)
C10	−0.10092 (12)	−0.30552 (17)	0.54594 (8)	0.0288 (4)
C11	−0.14158 (12)	−0.29491 (17)	0.60786 (8)	0.0306 (4)
C12	−0.23029 (14)	−0.38193 (19)	0.60570 (9)	0.0371 (4)
C13	0.62530 (12)	0.14409 (16)	0.16608 (8)	0.0253 (4)
C14	0.57282 (11)	0.03198 (16)	0.15376 (7)	0.0254 (4)
C15	0.53452 (11)	−0.00569 (15)	0.20800 (7)	0.0225 (3)
C16	0.55806 (10)	0.07908 (14)	0.26131 (7)	0.0198 (3)
C17	0.51565 (10)	0.06760 (14)	0.31758 (7)	0.0205 (3)
C18	0.61180 (10)	0.30603 (14)	0.42768 (7)	0.0206 (3)
C19	0.74920 (12)	0.42087 (16)	0.36876 (8)	0.0263 (4)
C20	0.83901 (11)	0.50861 (16)	0.37627 (8)	0.0251 (3)
C21	0.87886 (12)	0.49949 (17)	0.31384 (8)	0.0288 (4)
C22	0.96919 (12)	0.58270 (16)	0.31514 (9)	0.0292 (4)
C23	1.00835 (13)	0.56552 (19)	0.25291 (9)	0.0363 (4)
C24	1.09925 (15)	0.6467 (2)	0.25375 (11)	0.0456 (5)
H1	0.1857	0.1078	0.7232	0.0359*
H2	0.3076	0.2759	0.7585	0.0350*
H3	0.4065	0.3141	0.6763	0.0308*
H4	0.4322	0.2385	0.5686	0.0275*
H5	0.1756	−0.1728	0.5349	0.0339*
H6	0.1057	−0.0529	0.5062	0.0339*
H7	−0.0193	−0.2006	0.4487	0.0370*
H8	0.0502	−0.3187	0.4810	0.0370*
H9	−0.0268	−0.1312	0.5570	0.0347*
H10	0.0426	−0.2488	0.5892	0.0347*

H11	−0.1531	−0.2796	0.5064	0.0346*
H12	−0.0837	−0.3966	0.5398	0.0346*
H13	−0.0884	−0.3173	0.6475	0.0367*
H14	−0.1611	−0.2044	0.6129	0.0367*
H15	−0.2528	−0.3711	0.6468	0.0446*
H16	−0.2112	−0.4719	0.6016	0.0446*
H17	−0.2840	−0.3588	0.5673	0.0446*
H18	0.6560	0.1842	0.1349	0.0304*
H19	0.5633	−0.0152	0.1133	0.0305*
H20	0.4964	−0.0816	0.2081	0.0270*
H21	0.4735	−0.0047	0.3169	0.0247*
H22	0.7686	0.3308	0.3624	0.0316*
H23	0.6977	0.4468	0.3289	0.0316*
H24	0.8910	0.4824	0.4158	0.0301*
H25	0.8200	0.5987	0.3828	0.0301*
H26	0.8961	0.4085	0.3075	0.0345*
H27	0.8256	0.5246	0.2748	0.0345*
H28	1.0221	0.5602	0.3549	0.0350*
H29	0.9516	0.6743	0.3191	0.0350*
H30	1.0249	0.4736	0.2487	0.0436*
H31	0.9555	0.5888	0.2133	0.0436*
H32	1.1179	0.6370	0.2112	0.0547*
H33	1.1541	0.6181	0.2902	0.0547*
H34	1.0845	0.7374	0.2604	0.0547*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.01981 (7)	0.02133 (7)	0.01718 (6)	−0.00101 (4)	0.00858 (4)	0.00159 (4)
S1	0.0259 (2)	0.0329 (3)	0.02521 (19)	−0.00608 (15)	0.01238 (15)	0.00006 (16)
S2	0.0307 (2)	0.0315 (2)	0.02352 (18)	−0.00874 (16)	0.01346 (15)	−0.00467 (16)
S3	0.0328 (3)	0.0377 (3)	0.0294 (2)	−0.01495 (17)	0.01304 (17)	−0.00597 (17)
S4	0.02522 (19)	0.02514 (18)	0.02030 (17)	−0.00390 (14)	0.01060 (14)	−0.00137 (14)
S5	0.0295 (2)	0.0363 (3)	0.01867 (17)	−0.01023 (16)	0.01195 (15)	−0.00412 (15)
S6	0.0302 (2)	0.0334 (3)	0.02520 (19)	−0.01151 (16)	0.01289 (15)	−0.00660 (16)
N1	0.0205 (7)	0.0242 (7)	0.0208 (6)	−0.0019 (5)	0.0088 (5)	0.0025 (5)
N2	0.0218 (7)	0.0257 (7)	0.0238 (7)	−0.0040 (5)	0.0099 (5)	0.0003 (5)
N3	0.0207 (7)	0.0215 (7)	0.0192 (6)	−0.0007 (5)	0.0080 (5)	0.0022 (5)
N4	0.0210 (7)	0.0226 (7)	0.0215 (6)	−0.0029 (5)	0.0093 (5)	0.0008 (5)
C1	0.0302 (9)	0.0379 (10)	0.0258 (8)	0.0018 (7)	0.0152 (7)	0.0048 (7)
C2	0.0328 (9)	0.0345 (9)	0.0226 (8)	0.0041 (7)	0.0114 (7)	−0.0009 (7)
C3	0.0246 (8)	0.0290 (9)	0.0246 (8)	0.0001 (6)	0.0081 (6)	0.0002 (7)
C4	0.0186 (8)	0.0254 (8)	0.0220 (7)	0.0002 (6)	0.0077 (6)	0.0037 (6)
C5	0.0202 (8)	0.0266 (8)	0.0235 (7)	−0.0020 (6)	0.0084 (6)	0.0018 (6)
C6	0.0216 (8)	0.0251 (8)	0.0257 (8)	−0.0015 (6)	0.0090 (6)	0.0025 (6)
C7	0.0270 (9)	0.0329 (9)	0.0270 (8)	−0.0065 (7)	0.0109 (7)	0.0008 (7)
C8	0.0265 (9)	0.0356 (10)	0.0316 (9)	−0.0094 (7)	0.0095 (7)	0.0006 (7)
C9	0.0272 (9)	0.0296 (9)	0.0312 (9)	−0.0047 (7)	0.0096 (7)	0.0012 (7)

C10	0.0249 (9)	0.0336 (9)	0.0292 (8)	−0.0042 (7)	0.0087 (7)	0.0025 (7)
C11	0.0285 (9)	0.0339 (9)	0.0315 (9)	−0.0017 (7)	0.0113 (7)	0.0026 (7)
C12	0.0330 (10)	0.0471 (12)	0.0355 (10)	−0.0070 (8)	0.0162 (8)	0.0038 (8)
C13	0.0263 (9)	0.0325 (9)	0.0197 (7)	0.0015 (6)	0.0107 (6)	0.0005 (6)
C14	0.0248 (8)	0.0314 (9)	0.0210 (7)	0.0036 (6)	0.0074 (6)	−0.0051 (7)
C15	0.0216 (8)	0.0216 (8)	0.0251 (8)	0.0016 (6)	0.0072 (6)	−0.0021 (6)
C16	0.0186 (7)	0.0220 (8)	0.0198 (7)	0.0009 (6)	0.0066 (6)	0.0008 (6)
C17	0.0200 (8)	0.0209 (7)	0.0221 (7)	0.0005 (6)	0.0078 (6)	0.0020 (6)
C18	0.0201 (8)	0.0247 (8)	0.0181 (7)	−0.0005 (6)	0.0071 (6)	0.0025 (6)
C19	0.0263 (9)	0.0317 (9)	0.0239 (8)	−0.0073 (7)	0.0119 (6)	−0.0033 (7)
C20	0.0226 (8)	0.0268 (8)	0.0269 (8)	−0.0036 (6)	0.0083 (6)	−0.0009 (7)
C21	0.0270 (9)	0.0334 (9)	0.0286 (8)	−0.0058 (7)	0.0119 (7)	−0.0010 (7)
C22	0.0264 (9)	0.0294 (9)	0.0345 (9)	−0.0022 (7)	0.0127 (7)	0.0040 (7)
C23	0.0327 (10)	0.0436 (11)	0.0360 (10)	−0.0010 (8)	0.0150 (8)	0.0083 (8)
C24	0.0421 (12)	0.0488 (12)	0.0538 (13)	−0.0033 (9)	0.0271 (10)	0.0131 (10)

Geometric parameters (Å, º)

Pd1—S2	2.2946 (4)	C22—C23	1.523 (3)
Pd1—S5	2.2966 (4)	C23—C24	1.516 (3)
Pd1—N1	2.0278 (14)	C1—H1	0.950
Pd1—N3	2.0216 (14)	C2—H2	0.950
S1—C1	1.7122 (18)	C3—H3	0.950
S1—C4	1.7300 (17)	C5—H4	0.950
S2—C6	1.7360 (19)	C7—H5	0.990
S3—C6	1.7475 (16)	C7—H6	0.990
S3—C7	1.8129 (19)	C8—H7	0.990
S4—C13	1.7147 (18)	C8—H8	0.990
S4—C16	1.7320 (16)	C9—H9	0.990
S5—C18	1.7288 (17)	C9—H10	0.990
S6—C18	1.7498 (15)	C10—H11	0.990
S6—C19	1.8112 (19)	C10—H12	0.990
N1—N2	1.4009 (18)	C11—H13	0.990
N1—C5	1.3012 (19)	C11—H14	0.990
N2—C6	1.296 (2)	C12—H15	0.980
N3—N4	1.4029 (18)	C12—H16	0.980
N3—C17	1.3026 (19)	C12—H17	0.980
N4—C18	1.2985 (19)	C13—H18	0.950
C1—C2	1.362 (3)	C14—H19	0.950
C2—C3	1.409 (3)	C15—H20	0.950
C3—C4	1.381 (3)	C17—H21	0.950
C4—C5	1.435 (3)	C19—H22	0.990
C7—C8	1.529 (3)	C19—H23	0.990
C8—C9	1.522 (3)	C20—H24	0.990
C9—C10	1.524 (3)	C20—H25	0.990
C10—C11	1.523 (3)	C21—H26	0.990
C11—C12	1.521 (3)	C21—H27	0.990
C13—C14	1.364 (3)	C22—H28	0.990

C14—C15	1.408 (3)	C22—H29	0.990
C15—C16	1.386 (2)	C23—H30	0.990
C16—C17	1.430 (3)	C23—H31	0.990
C19—C20	1.523 (3)	C24—H32	0.980
C20—C21	1.525 (3)	C24—H33	0.980
C21—C22	1.520 (3)	C24—H34	0.980

S1···N1	3.3418 (15)	C22···H13^{iii}	3.2117
S1···N2	2.8431 (15)	C22···H16^{iii}	3.5813
S1···C7	3.4705 (16)	C23···H1^{xvi}	3.2288
S2···C17	3.2595 (16)	C23···H13^{iii}	3.3178
S4···N3	3.3245 (15)	C23···H13^{xvi}	3.4597
S4···N4	2.8340 (14)	C23···H14^{xvi}	3.5676
S4···C19	3.5184 (16)	C24···H1^{xvi}	3.0297
S5···C5	3.2970 (17)	C24···H10^{xvi}	3.4675
N2···C4	2.792 (2)	C24···H13^{xvi}	3.4659
N2···C7	2.833 (3)	C24···H16^{iii}	3.5220
N4···C16	2.7909 (19)	C24···H26^{xvii}	3.0049
N4···C19	2.848 (3)	H1···C12^{xiv}	3.4422
C5···C6	3.407 (2)	H1···C23^{x}	3.2288
C17···C18	3.409 (2)	H1···C24^{x}	3.0297
S5···C13^{i}	3.5849 (17)	H1···H13^{xiv}	3.3644
N4···C15^{ii}	3.4088 (19)	H1···H15^{xiv}	2.6333
C2···C15^{iii}	3.380 (3)	H1···H29^{ix}	2.9526
C3···C15^{i}	3.583 (3)	H1···H30^{x}	2.5613
C3···C16^{i}	3.466 (2)	H1···H32^{x}	2.6989
C4···C17^{iii}	3.371 (2)	H1···H33^{x}	2.8102
C12···C14^{iv}	3.496 (3)	H2···S2^{i}	3.4900
C13···S5^{v}	3.5849 (17)	H2···N3^{i}	3.4500
C14···C12^{vi}	3.496 (3)	H2···C15^{iii}	3.5252
C14···C18^{vii}	3.584 (2)	H2···C17^{i}	3.2861
C15···N4^{vii}	3.4088 (19)	H2···C21^{ix}	3.5401
C15···C2^{iii}	3.380 (3)	H2···H15^{xiv}	2.7305
C15···C3^{v}	3.583 (3)	H2···H20^{iii}	3.3270
C16···C3^{v}	3.466 (2)	H2···H21^{i}	3.3273
C17···C4^{iii}	3.371 (2)	H2···H23^{ix}	3.3893
C18···C14^{ii}	3.584 (2)	H2···H25^{ix}	3.2994
Pd1···H4	2.9696	H2···H27^{ix}	2.7526
Pd1···H21	2.9724	H3···S4^{i}	3.0909
S1···H2	3.4858	H3···C13^{i}	3.1313
S1···H3	3.4814	H3···C14^{i}	2.9389
S1···H5	3.0957	H3···C15^{i}	2.6439
S1···H6	2.9150	H3···C16^{i}	2.6419
S2···H21	2.6304	H3···C17^{i}	3.1953
S3···H7	2.8693	H3···C19^{ix}	3.4854
S3···H8	2.9142	H3···H19^{i}	3.4877
S4···H19	3.4855	H3···H20^{iii}	3.4360
S4···H20	3.4875	H3···H20^{i}	3.0498

S4···H22	3.0257	H3···H21^{i}	3.4528
S4···H23	3.0792	H3···H23^{ix}	2.8625
S5···H4	2.6192	H3···H25^{ix}	3.2225
S6···H24	2.8956	H4···C13^{i}	3.1867
S6···H25	2.8886	H4···C14^{i}	3.3075
N2···H4	3.1232	H4···H17^{viii}	3.3036
N2···H5	2.7608	H4···H18^{i}	3.1878
N2···H6	2.6580	H4···H19^{i}	3.4071
N4···H21	3.1249	H4···H21^{iii}	3.4222
N4···H22	2.6265	H5···S6^{iii}	3.1605
N4···H23	2.8304	H5···N4^{iii}	3.3533
C1···H3	3.1885	H5···C18^{iii}	3.1863
C3···H1	3.1958	H5···C19^{iii}	3.2680
C3···H4	2.5861	H5···H22^{iii}	2.6473
C4···H1	3.3984	H5···H24^{iii}	3.5593
C4···H2	3.2291	H6···C8^{viii}	3.5089
C5···H3	2.6918	H6···C9^{viii}	3.2418
C6···H5	2.9209	H6···H6^{viii}	3.0917
C6···H6	2.8724	H6···H7^{viii}	3.1253
C7···H9	2.6794	H6···H9^{viii}	2.4221
C7···H10	2.6776	H6···H11^{viii}	3.5336
C8···H11	2.7413	H7···S1^{viii}	3.2784
C8···H12	2.7544	H7···C22^{xi}	3.5349
C9···H5	2.7172	H7···H6^{viii}	3.1253
C9···H6	2.6768	H7···H9^{viii}	3.5087
C9···H13	2.7042	H7···H24^{xi}	3.5259
C9···H14	2.7367	H7···H25^{xi}	3.1185
C10···H7	2.7585	H7···H28^{xi}	3.2850
C10···H8	2.7570	H7···H29^{xi}	2.9169
C10···H15	3.3757	H8···C20^{iii}	3.5745
C10···H16	2.7405	H8···C22^{xi}	3.4935
C10···H17	2.7438	H8···H12^{xviii}	3.0374
C11···H9	2.7101	H8···H22^{iii}	3.5959
C11···H10	2.7236	H8···H24^{xi}	3.0889
C12···H11	2.7475	H8···H24^{iii}	2.6960
C12···H12	2.7152	H8···H25^{xi}	3.4608
C13···H20	3.1943	H8···H28^{xi}	2.8339
C15···H18	3.2011	H8···H29^{xi}	3.2971
C15···H21	2.5893	H9···S3^{viii}	3.5632
C16···H18	3.4035	H9···C7^{viii}	3.2183
C16···H19	3.2289	H9···H6^{viii}	2.4221
C17···H20	2.7017	H9···H7^{viii}	3.5087
C18···H22	2.8400	H9···H31^{x}	3.3269
C18···H23	2.9836	H9···H32^{x}	3.3361
C19···H26	2.6525	H10···C19^{iii}	3.3349
C19···H27	2.6549	H10···C20^{iii}	3.1501
C20···H28	2.7408	H10···C21^{iii}	3.3050
C20···H29	2.7747	H10···C24^{x}	3.4675

C21···H22	2.6760	H10···H22^{iii}	2.7133
C21···H23	2.6696	H10···H24^{iii}	2.6043
C21···H30	2.7073	H10···H26^{iii}	2.6746
C21···H31	2.7173	H10···H31^{x}	3.5067
C22···H24	2.7716	H10···H32^{x}	2.7450
C22···H25	2.7736	H10···H34^{x}	3.4467
C22···H32	3.3693	H11···S1^{viii}	3.4028
C22···H33	2.7665	H11···N1^{viii}	3.3602
C22···H34	2.7033	H11···N2^{viii}	3.2004
C23···H26	2.6868	H11···C4^{viii}	3.2546
C23···H27	2.7217	H11···C5^{viii}	3.3018
C24···H28	2.7215	H11···C20^{xi}	3.4550
C24···H29	2.7313	H11···H6^{viii}	3.5336
H1···H2	2.4205	H11···H24^{xi}	3.2465
H2···H3	2.4633	H11···H25^{xi}	2.7928
H3···H4	2.4651	H12···C20^{xi}	3.4358
H5···H7	2.8775	H12···C22^{iii}	3.5990
H5···H8	2.3749	H12···H8^{xviii}	3.0374
H5···H9	2.9917	H12···H24^{xi}	2.8004
H5···H10	2.5112	H12···H24^{iii}	2.7630
H6···H7	2.4055	H12···H25^{xi}	3.1993
H6···H8	2.8773	H12···H26^{iii}	3.5798
H6···H9	2.4695	H12···H28^{iii}	2.7303
H6···H10	2.9278	H13···C21^{iii}	3.4046
H7···H9	2.3769	H13···C22^{iii}	3.2117
H7···H10	2.8659	H13···C23^{iii}	3.3178
H7···H11	2.5749	H13···C23^{x}	3.4597
H7···H12	3.0488	H13···C24^{x}	3.4659
H8···H9	2.8660	H13···H1^{xv}	3.3644
H8···H10	2.3779	H13···H26^{iii}	2.7793
H8···H11	3.0261	H13···H28^{iii}	2.6889
H8···H12	2.5874	H13···H30^{iii}	2.6645
H9···H11	2.3801	H13···H31^{x}	2.7275
H9···H12	2.8629	H13···H32^{x}	3.4140
H9···H13	2.9547	H13···H33^{iii}	3.5777
H9···H14	2.5379	H13···H34^{x}	3.0357
H10···H11	2.8629	H14···S2^{viii}	3.3048
H10···H12	2.3694	H14···N1^{viii}	3.4150
H10···H13	2.5174	H14···N2^{viii}	3.1380
H10···H14	3.0255	H14···C6^{viii}	2.9635
H11···H13	2.8634	H14···C23^{x}	3.5676
H11···H14	2.3623	H14···H31^{x}	2.5993
H11···H16	3.0448	H15···C1^{xv}	3.1528
H11···H17	2.5836	H15···C2^{xv}	3.1957
H12···H13	2.3883	H15···C13^{iv}	3.3734
H12···H14	2.8633	H15···C14^{iv}	2.9762
H12···H16	2.5456	H15···H1^{xv}	2.6333
H12···H17	3.0003	H15···H2^{xv}	2.7305

H13···H15	2.3509	H15···H18^{iv}	3.4739
H13···H16	2.3687	H15···H19^{iv}	2.7505
H13···H17	2.8573	H15···H30^{iii}	3.5427
H14···H15	2.3535	H15···H33^{iii}	3.0479
H14···H16	2.8573	H16···S6^{xi}	3.3910
H14···H17	2.3662	H16···C13^{iv}	3.4054
H18···H19	2.4215	H16···C14^{iv}	3.4837
H19···H20	2.4607	H16···C22^{iii}	3.5813
H20···H21	2.4778	H16···C24^{iii}	3.5220
H22···H24	2.3848	H16···H18^{iv}	3.0573
H22···H25	2.8757	H16···H19^{iv}	3.2074
H22···H26	2.4585	H16···H28^{iii}	2.7255
H22···H27	2.9381	H16···H30^{iii}	3.5247
H23···H24	2.8758	H16···H33^{iii}	2.6597
H23···H25	2.3896	H17···Pd1^{viii}	3.2712
H23···H26	2.9249	H17···S6^{xi}	3.3568
H23···H27	2.4542	H17···N1^{viii}	3.0547
H24···H26	2.3816	H17···C5^{viii}	3.2805
H24···H27	2.8690	H17···C14^{iv}	3.4790
H24···H28	2.5819	H17···H4^{viii}	3.3036
H24···H29	3.0793	H17···H19^{iv}	2.8466
H25···H26	2.8688	H18···S2^{ii}	3.1489
H25···H27	2.3798	H18···S3^{ii}	3.4390
H25···H28	3.0302	H18···S5^{v}	2.9879
H25···H29	2.6205	H18···H4^{v}	3.1878
H26···H28	2.3841	H18···H15^{vi}	3.4739
H26···H29	2.8586	H18···H16^{vi}	3.0573
H26···H30	2.4895	H18···H33^{xii}	2.8069
H26···H31	2.9591	H19···S5^{vii}	3.1461
H27···H28	2.8588	H19···S5^{v}	3.4501
H27···H29	2.3564	H19···N4^{vii}	3.4351
H27···H30	2.9976	H19···C12^{vi}	3.1035
H27···H31	2.5375	H19···C18^{vii}	3.0160
H28···H30	2.3806	H19···H3^{v}	3.4877
H28···H31	2.8650	H19···H4^{v}	3.4071
H28···H33	2.5885	H19···H15^{vi}	2.7505
H28···H34	2.9610	H19···H16^{vi}	3.2074
H29···H30	2.8649	H19···H17^{vi}	2.8466
H29···H31	2.3728	H20···S4^{vii}	3.1330
H29···H32	3.5998	H20···N3^{vii}	3.2668
H29···H33	3.0721	H20···N4^{vii}	2.6186
H29···H34	2.5301	H20···C2^{iii}	3.2749
H30···H32	2.3730	H20···C3^{iii}	3.3409
H30···H33	2.3387	H20···C18^{vii}	3.0763
H30···H34	2.8534	H20···C19^{vii}	3.4030
H31···H32	2.3244	H20···H2^{iii}	3.3270
H31···H33	2.8523	H20···H3^{iii}	3.4360
H31···H34	2.3883	H20···H3^{v}	3.0498

Pd1···H17^{viii}	3.2712	H20···H23^{vii}	2.6390
S1···H7^{viii}	3.2784	H21···S4^{vii}	3.4439
S1···H11^{viii}	3.4028	H21···C3^{iii}	3.4632
S1···H25^{ix}	3.5060	H21···C4^{iii}	3.2699
S1···H32^{x}	3.4718	H21···C5^{iii}	3.3439
S2···H2^{v}	3.4900	H21···H2^{v}	3.3273
S2···H14^{viii}	3.3048	H21···H3^{v}	3.4528
S2···H18^{vii}	3.1489	H21···H4^{iii}	3.4222
S2···H27^{vii}	3.4367	H21···H23^{vii}	3.3985
S3···H9^{viii}	3.5632	H22···C7^{iii}	3.5324
S3···H18^{vii}	3.4390	H22···C9^{iii}	3.5893
S3···H34^{xi}	3.4824	H22···H5^{iii}	2.6473
S4···H3^{v}	3.0909	H22···H8^{iii}	3.5959
S4···H20^{ii}	3.1330	H22···H10^{iii}	2.7133
S4···H21^{ii}	3.4439	H22···H32^{xii}	3.1633
S4···H32^{xii}	3.4790	H23···C2^{ix}	3.4935
S4···H33^{xii}	3.3714	H23···C3^{ix}	3.2174
S5···H18^{i}	2.9879	H23···C15^{ii}	3.1741
S5···H19^{ii}	3.1461	H23···H2^{ix}	3.3893
S5···H19^{i}	3.4501	H23···H3^{ix}	2.8625
S6···H5^{iii}	3.1605	H23···H20^{ii}	2.6390
S6···H16^{xiii}	3.3910	H23···H21^{ii}	3.3985
S6···H17^{xiii}	3.3568	H24···C8^{iii}	3.3152
N1···H11^{viii}	3.3602	H24···C9^{iii}	3.1571
N1···H14^{viii}	3.4150	H24···C10^{xiii}	3.4566
N1···H17^{viii}	3.0547	H24···C10^{iii}	3.3774
N2···H11^{viii}	3.2004	H24···H5^{iii}	3.5593
N2···H14^{viii}	3.1380	H24···H7^{xiii}	3.5259
N3···H2^{v}	3.4500	H24···H8^{xiii}	3.0889
N3···H20^{ii}	3.2668	H24···H8^{iii}	2.6960
N4···H5^{iii}	3.3533	H24···H10^{iii}	2.6043
N4···H19^{ii}	3.4351	H24···H11^{xiii}	3.2465
N4···H20^{ii}	2.6186	H24···H12^{xiii}	2.8004
C1···H15^{xiv}	3.1528	H24···H12^{iii}	2.7630
C1···H25^{ix}	3.2136	H25···S1^{ix}	3.5060
C1···H29^{ix}	3.1652	H25···C1^{ix}	3.2136
C1···H30^{x}	3.4653	H25···C2^{ix}	2.9267
C1···H32^{x}	3.2726	H25···C3^{ix}	2.8789
C1···H33^{x}	3.5584	H25···C4^{ix}	3.1567
C2···H15^{xiv}	3.1957	H25···C10^{xiii}	3.4317
C2···H20^{iii}	3.2749	H25···H2^{ix}	3.2994
C2···H23^{ix}	3.4935	H25···H3^{ix}	3.2225
C2···H25^{ix}	2.9267	H25···H7^{xiii}	3.1185
C2···H27^{ix}	3.1038	H25···H8^{xiii}	3.4608
C2···H29^{ix}	3.5271	H25···H11^{xiii}	2.7928
C3···H20^{iii}	3.3409	H25···H12^{xiii}	3.1993
C3···H21^{iii}	3.4632	H26···C9^{iii}	3.5613
C3···H23^{ix}	3.2174	H26···C24^{xii}	3.0049

C3···H25^{ix}	2.8789	H26···H10^{iii}	2.6746
C4···H11^{viii}	3.2546	H26···H12^{iii}	3.5798
C4···H21^{iii}	3.2699	H26···H13^{iii}	2.7793
C4···H25^{ix}	3.1567	H26···H32^{xii}	2.8442
C5···H11^{viii}	3.3018	H26···H34^{xii}	2.3188
C5···H17^{viii}	3.2805	H27···S2^{ii}	3.4367
C5···H21^{iii}	3.3439	H27···C2^{ix}	3.1038
C6···H14^{viii}	2.9635	H27···H2^{ix}	2.7526
C7···H9^{viii}	3.2183	H27···H34^{xii}	3.3783
C7···H22^{iii}	3.5324	H28···C8^{xiii}	3.4988
C8···H6^{viii}	3.5089	H28···C10^{iii}	3.3624
C8···H24^{iii}	3.3152	H28···C11^{iii}	3.2120
C8···H28^{xi}	3.4988	H28···C12^{iii}	3.3673
C8···H29^{xi}	3.5517	H28···H7^{xiii}	3.2850
C9···H6^{viii}	3.2418	H28···H8^{xiii}	2.8339
C9···H22^{iii}	3.5893	H28···H12^{iii}	2.7303
C9···H24^{iii}	3.1571	H28···H13^{iii}	2.6889
C9···H26^{iii}	3.5613	H28···H16^{iii}	2.7255
C9···H32^{x}	3.4914	H29···C1^{ix}	3.1652
C10···H24^{xi}	3.4566	H29···C2^{ix}	3.5271
C10···H24^{iii}	3.3774	H29···C8^{xiii}	3.5517
C10···H25^{xi}	3.4317	H29···H1^{ix}	2.9526
C10···H28^{iii}	3.3624	H29···H7^{xiii}	2.9169
C11···H28^{iii}	3.2120	H29···H8^{xiii}	3.2971
C11···H30^{iii}	3.5414	H29···H30^{xvii}	3.4539
C11···H31^{x}	3.1188	H30···C1^{xvi}	3.4653
C12···H1^{xv}	3.4422	H30···C11^{iii}	3.5414
C12···H19^{iv}	3.1035	H30···H1^{xvi}	2.5613
C12···H28^{iii}	3.3673	H30···H13^{iii}	2.6645
C12···H33^{iii}	3.2650	H30···H15^{iii}	3.5427
C13···H3^{v}	3.1313	H30···H16^{iii}	3.5247
C13···H4^{v}	3.1867	H30···H29^{xii}	3.4539
C13···H15^{vi}	3.3734	H30···H34^{xii}	2.8670
C13···H16^{vi}	3.4054	H31···C11^{xvi}	3.1188
C13···H33^{xii}	2.9959	H31···H9^{xvi}	3.3269
C14···H3^{v}	2.9389	H31···H10^{xvi}	3.5067
C14···H4^{v}	3.3075	H31···H13^{xvi}	2.7275
C14···H15^{vi}	2.9762	H31···H14^{xvi}	2.5993
C14···H16^{vi}	3.4837	H32···S1^{xvi}	3.4718
C14···H17^{vi}	3.4790	H32···S4^{xvii}	3.4790
C15···H2^{iii}	3.5252	H32···C1^{xvi}	3.2726
C15···H3^{v}	2.6439	H32···C9^{xvi}	3.4914
C15···H23^{vii}	3.1741	H32···H1^{xvi}	2.6989
C16···H3^{v}	2.6419	H32···H9^{xvi}	3.3361
C17···H2^{v}	3.2861	H32···H10^{xvi}	2.7450
C17···H3^{v}	3.1953	H32···H13^{xvi}	3.4140
C18···H5^{iii}	3.1863	H32···H22^{xvii}	3.1633
C18···H19^{ii}	3.0160	H32···H26^{xvii}	2.8442

C18···H20^{ii}	3.0763	H33···S4^{xvii}	3.3714
C19···H3^{ix}	3.4854	H33···C1^{xvi}	3.5584
C19···H5^{iii}	3.2680	H33···C12^{iii}	3.2650
C19···H10^{iii}	3.3349	H33···C13^{xvii}	2.9959
C19···H20^{ii}	3.4030	H33···H1^{xvi}	2.8102
C20···H8^{iii}	3.5745	H33···H13^{iii}	3.5777
C20···H10^{iii}	3.1501	H33···H15^{iii}	3.0479
C20···H11^{xiii}	3.4550	H33···H16^{iii}	2.6597
C20···H12^{xiii}	3.4358	H33···H18^{xvii}	2.8069
C21···H2^{ix}	3.5401	H34···S3^{xiii}	3.4824
C21···H10^{iii}	3.3050	H34···C21^{xvii}	3.2219
C21···H13^{iii}	3.4046	H34···H10^{xvi}	3.4467
C21···H34^{xii}	3.2219	H34···H13^{xvi}	3.0357
C22···H7^{xiii}	3.5349	H34···H26^{xvii}	2.3188
C22···H8^{xiii}	3.4935	H34···H27^{xvii}	3.3783
C22···H12^{iii}	3.5990	H34···H30^{xvii}	2.8670

S2—Pd1—S5	174.706 (15)	C7—C8—H8	109.534
S2—Pd1—N1	83.13 (4)	C9—C8—H7	109.539
S2—Pd1—N3	96.37 (4)	C9—C8—H8	109.538
S5—Pd1—N1	97.55 (4)	H7—C8—H8	108.094
S5—Pd1—N3	82.95 (4)	C8—C9—H9	108.735
N1—Pd1—N3	179.49 (5)	C8—C9—H10	108.728
C1—S1—C4	91.38 (9)	C10—C9—H9	108.723
Pd1—S2—C6	95.85 (5)	C10—C9—H10	108.731
C6—S3—C7	101.58 (8)	H9—C9—H10	107.649
C13—S4—C16	91.46 (8)	C9—C10—H11	109.041
Pd1—S5—C18	95.86 (5)	C9—C10—H12	109.039
C18—S6—C19	102.16 (8)	C11—C10—H11	109.048
Pd1—N1—N2	121.37 (10)	C11—C10—H12	109.046
Pd1—N1—C5	124.60 (11)	H11—C10—H12	107.808
N2—N1—C5	114.02 (14)	C10—C11—H13	108.912
N1—N2—C6	113.05 (14)	C10—C11—H14	108.907
Pd1—N3—N4	121.36 (10)	C12—C11—H13	108.921
Pd1—N3—C17	124.52 (11)	C12—C11—H14	108.922
N4—N3—C17	114.04 (13)	H13—C11—H14	107.746
N3—N4—C18	112.79 (13)	C11—C12—H15	109.461
S1—C1—C2	112.92 (15)	C11—C12—H16	109.469
C1—C2—C3	111.69 (16)	C11—C12—H17	109.480
C2—C3—C4	113.50 (15)	H15—C12—H16	109.467
S1—C4—C3	110.51 (13)	H15—C12—H17	109.471
S1—C4—C5	127.64 (12)	H16—C12—H17	109.479
C3—C4—C5	121.82 (15)	S4—C13—H18	123.669
N1—C5—C4	129.63 (15)	C14—C13—H18	123.665
S2—C6—S3	113.85 (9)	C13—C14—H19	123.956
S2—C6—N2	126.31 (13)	C15—C14—H19	123.944
S3—C6—N2	119.83 (14)	C14—C15—H20	123.386
S3—C7—C8	110.55 (11)	C16—C15—H20	123.364

C7—C8—C9	110.55 (14)	N3—C17—H21	115.283
C8—C9—C10	114.09 (14)	C16—C17—H21	115.291
C9—C10—C11	112.74 (14)	S6—C19—H22	109.524
C10—C11—C12	113.29 (14)	S6—C19—H23	109.519
S4—C13—C14	112.67 (14)	C20—C19—H22	109.527
C13—C14—C15	112.10 (14)	C20—C19—H23	109.533
C14—C15—C16	113.25 (14)	H22—C19—H23	108.099
S4—C16—C15	110.52 (12)	C19—C20—H24	109.789
S4—C16—C17	127.07 (11)	C19—C20—H25	109.788
C15—C16—C17	121.93 (14)	C21—C20—H24	109.784
N3—C17—C16	129.43 (14)	C21—C20—H25	109.775
S5—C18—S6	114.03 (8)	H24—C20—H25	108.238
S5—C18—N4	126.29 (12)	C20—C21—H26	108.594
S6—C18—N4	119.68 (13)	C20—C21—H27	108.600
S6—C19—C20	110.60 (12)	C22—C21—H26	108.603
C19—C20—C21	109.45 (13)	C22—C21—H27	108.597
C20—C21—C22	114.67 (14)	H26—C21—H27	107.562
C21—C22—C23	112.39 (14)	C21—C22—H28	109.116
C22—C23—C24	113.10 (16)	C21—C22—H29	109.120
S1—C1—H1	123.545	C23—C22—H28	109.128
C2—C1—H1	123.538	C23—C22—H29	109.124
C1—C2—H2	124.148	H28—C22—H29	107.857
C3—C2—H2	124.162	C22—C23—H30	108.950
C2—C3—H3	123.244	C22—C23—H31	108.957
C4—C3—H3	123.254	C24—C23—H30	108.964
N1—C5—H4	115.179	C24—C23—H31	108.970
C4—C5—H4	115.195	H30—C23—H31	107.768
S3—C7—H5	109.538	C23—C24—H32	109.466
S3—C7—H6	109.533	C23—C24—H33	109.479
C8—C7—H5	109.539	C23—C24—H34	109.476
C8—C7—H6	109.535	H32—C24—H33	109.469
H5—C7—H6	108.101	H32—C24—H34	109.466
C7—C8—H7	109.541	H33—C24—H34	109.471

S2—Pd1—N1—N2	5.37 (8)	N2—N1—C5—C4	0.9 (2)
S2—Pd1—N1—C5	−175.96 (9)	C5—N1—N2—C6	176.43 (11)
N1—Pd1—S2—C6	−3.71 (4)	N1—N2—C6—S2	0.40 (19)
S2—Pd1—N3—N4	166.01 (8)	N1—N2—C6—S3	−178.57 (10)
S2—Pd1—N3—C17	−10.48 (9)	Pd1—N3—N4—C18	8.32 (14)
N3—Pd1—S2—C6	176.34 (4)	Pd1—N3—C17—C16	170.50 (9)
S5—Pd1—N1—N2	−179.93 (8)	N4—N3—C17—C16	−6.22 (19)
S5—Pd1—N1—C5	−1.25 (9)	C17—N3—N4—C18	−174.84 (11)
N1—Pd1—S5—C18	−174.28 (4)	N3—N4—C18—S5	−1.78 (18)
S5—Pd1—N3—N4	−8.71 (8)	N3—N4—C18—S6	178.39 (9)
S5—Pd1—N3—C17	174.80 (9)	S1—C1—C2—C3	0.21 (18)
N3—Pd1—S5—C18	5.62 (4)	C1—C2—C3—C4	−0.05 (19)
C1—S1—C4—C3	0.20 (11)	C2—C3—C4—S1	−0.12 (17)
C1—S1—C4—C5	178.48 (13)	C2—C3—C4—C5	−178.52 (12)

C4—S1—C1—C2	−0.24 (12)	S1—C4—C5—N1	2.6 (3)
Pd1—S2—C6—S3	−177.88 (7)	C3—C4—C5—N1	−179.33 (14)
Pd1—S2—C6—N2	3.09 (13)	S3—C7—C8—C9	−177.26 (9)
C6—S3—C7—C8	177.07 (9)	C7—C8—C9—C10	−179.89 (12)
C7—S3—C6—S2	178.73 (9)	C8—C9—C10—C11	−179.07 (12)
C7—S3—C6—N2	−2.17 (13)	C9—C10—C11—C12	−177.74 (12)
C13—S4—C16—C15	0.99 (10)	S4—C13—C14—C15	0.50 (17)
C13—S4—C16—C17	−171.07 (11)	C13—C14—C15—C16	0.27 (18)
C16—S4—C13—C14	−0.86 (11)	C14—C15—C16—S4	−0.90 (16)
Pd1—S5—C18—S6	175.85 (7)	C14—C15—C16—C17	171.64 (12)
Pd1—S5—C18—N4	−3.99 (12)	S4—C16—C17—N3	−5.3 (2)
C18—S6—C19—C20	−171.22 (9)	C15—C16—C17—N3	−176.58 (13)
C19—S6—C18—S5	177.78 (8)	S6—C19—C20—C21	−179.57 (9)
C19—S6—C18—N4	−2.37 (12)	C19—C20—C21—C22	−179.85 (12)
Pd1—N1—N2—C6	−4.76 (15)	C20—C21—C22—C23	177.59 (12)
Pd1—N1—C5—C4	−177.83 (9)	C21—C22—C23—C24	−179.31 (12)

Symmetry codes: (i) x, $-y+1/2$, $z+1/2$; (ii) $-x+1$, $y+1/2$, $-z+1/2$; (iii) $-x+1$, $-y$, $-z+1$; (iv) $x-1$, $-y-1/2$, $z+1/2$; (v) x, $-y+1/2$, $z-1/2$; (vi) $x+1$, $-y-1/2$, $z-1/2$; (vii) $-x+1$, $y-1/2$, $-z+1/2$; (viii) $-x$, $-y$, $-z+1$; (ix) $-x+1$, $-y+1$, $-z+1$; (x) $x-1$, $-y+1/2$, $z+1/2$; (xi) $x-1$, $y-1$, z; (xii) $-x+2$, $y-1/2$, $-z+1/2$; (xiii) $x+1$, $y+1$, z; (xiv) $-x$, $y+1/2$, $-z+3/2$; (xv) $-x$, $y-1/2$, $-z+3/2$; (xvi) $x+1$, $-y+1/2$, $z-1/2$; (xvii) $-x+2$, $y+1/2$, $-z+1/2$; (xviii) $-x$, $-y-1$, $-z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H4···S5	0.95	2.62	3.2970 (17)	129
C15—H20···N4^{vii}	0.95	2.62	3.4088 (19)	141
C17—H21···S2	0.95	2.63	3.2596 (16)	124

Symmetry code: (vii) $-x+1$, $y-1/2$, $-z+1/2$.