Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dipotassium tetrakis(thiocyanato-κS)-palladate(II)–(2,2′-bipyrimidine-$\kappa^2N^1,N^{1'}$)bis(thiocyanato-κS)-palladium(II) (1/2)

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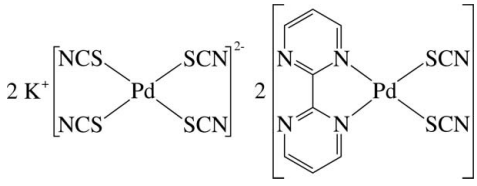
Received 3 April 2012; accepted 8 April 2012

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.080; data-to-parameter ratio = 15.3.

The asymmetric unit of the title compound, $K_2[Pd(NCS)_4]\cdot 2[Pd(NCS)_2(C_8H_6N_4)]$, contains two crystallographically independent half-molecules of the anionic Pd^{II} complex, two K^+ cations and two independent neutral Pd^{II} complexes; an inversion centre is located at the centroid of each anionic complex. In the anionic complexes, each Pd^{II} ion is four-coordinated in an almost regular square-planar environment by four S atoms from four SCN^- anions, and the PdS_4 unit is exactly planar. In the neutral complexes, the Pd^{II} ion has a slightly distorted square-planar coordination environment defined by two pyrimidine N atoms derived from a chelating 2,2′-bipyrimidine ligand and two mutually *cis* S atoms from two SCN^- anions. Both 2,2′-bipyrimidine ligands are almost planar [dihedral angle between the rings = 3.98 (16) and 4.57 (17)°] and also chelate to a potassium ion from their other two N atoms. In the crystal, the K^+ ions interact with various S and N atoms of the ligands, forming a three-dimensional polymeric network, in which the shortest K···K contacts between the KN_7S polyhedra are 4.4389 (17) and 4.4966 (18) Å. Intra- and intermolecular C—H···S and C—H···N hydrogen bonds are also observed.

Related literature

For the crystal structure of $K_2[Pd(SCN)_4]$, see: Mawby & Pringle (1972); Ha (2010).



Experimental

Crystal data

$K_2[Pd(NCS)_4]\cdot 2[Pd(NCS)_2(C_8H_6N_4)]$
M_r = 1178.38
Monoclinic, $P2_1/c$
a = 15.9625 (7) Å
b = 10.9700 (5) Å
c = 21.6801 (9) Å
β = 94.104 (1)°
V = 3786.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.12 mm^{-1}
T = 200 K
0.28 × 0.24 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.854, T_{max} = 1.000
22881 measured reflections
7371 independent reflections
5722 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.08
7371 reflections
481 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pd1—N1	2.074 (3)	Pd2—S3^{i}	2.2958 (10)
Pd1—N4	2.070 (3)	Pd2—S4	2.2829 (11)
Pd1—S1	2.2945 (11)	Pd3—S5	2.3388 (9)
Pd1—S2	2.3077 (11)	Pd3—S6	2.3314 (9)
Pd2—N7	2.059 (3)	Pd4—S7	2.3157 (10)
Pd2—N10	2.069 (3)	Pd4—S8	2.3419 (10)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···S1	0.95	2.77	3.334 (4)	119
C1—H1···N11^{ii}	0.95	2.45	3.134 (5)	128
C6—H6···S7^{iii}	0.95	2.76	3.457 (4)	131
C8—H8···S2	0.95	2.77	3.321 (4)	118
C11—H11···S3^{i}	0.95	2.82	3.371 (4)	118
C11—H11···N6^{iv}	0.95	2.63	3.315 (5)	130
C13—H13···N15^{v}	0.95	2.61	3.376 (5)	138
C16—H16···S6^{ii}	0.95	2.83	3.640 (4)	144
C18—H18···S4	0.95	2.71	3.276 (4)	119

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Priority Research Centers Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (2011–0030747).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6728).

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supplementary materials

Acta Cryst. (2012). E**68**, m616–m617 [doi:10.1107/S1600536812015383]

Dipotassium tetrakis(thiocyanato-κS)palladate(II)–(2,2′-bipyrimidine-$\kappa^2N^1,N^{1'}$)bis(thiocyanato-κS)palladium(II) (1/2)

Kwang Ha

Comment

The title compound, $K_2[Pd(SCN)_4].2[Pd(SCN)_2(bpym)]$ (bpym = 2,2′-bipyrimidine), was unexpected obtained from the reaction of Na_2PdCl_4 with KSCN and bpym. The asymmetric unit contains two crystallographically independent half-molecules of the anionic Pd^{II} complex $[Pd(SCN)_4]^{2-}$, two K^+ cations and two independent neutral Pd^{II} complexes $[Pd(SCN)_2(bpym)]$; an inversion centre is located at the centroid of each anionic complex (Fig. 1). The crystal structure of $K_2[Pd(SCN)_4]$ has been investigated previously (Mawby & Pringle, 1972; Ha, 2010).

In the anionic complexes, each Pd^{II} ion is four-coordinated in an essentially square-planar environment by four S atoms from four SCN^- anions, and the PdS_4 unit is exactly planar. The two complexes are chemically identical, but slightly different in geometry. The Pd—S bond lengths are roughly equal [Pd—S: 2.3157 (10)–2.3419 (10) Å] (Table 1). The thiocyanato ligands are almost linear displaying S—C—N bond angles of 174.8 (4)°–178.1 (4)°, and the S atoms coordinate to the Pd atom with the nearly tetrahedral Pd—S—C bond angles of 106.57 (13)°–110.44 (13)°.

In the two neutral complexes, each Pd^{II} ion has a slightly distorted square-planar coordination environment defined by two pyrimidine N atoms derived from a chelating bpym ligand and two mutually *cis* S atoms from two SCN^- anions. The complexes are fairly different in geometry, because the coordination modes of the anions are significantly different. The two thiocyanato ligands are located on the same side of the PdS_2N_2 unit plane in the complex with Pd1, whereas in the other complex with Pd2, the ligands lie on the opposite sides of the PdS_2N_2 unit. But, the Pd—N and Pd—S bond lengths are nearly equivalent, respectively [Pd—N = 2.059 (3)–2.074 (3) Å; Pd—S = 2.2829 (11)–2.3077 (11) Å] (Table 1). The bpym ligands are slightly inclined to the least-squares plane of the PdS_2N_2 unit [maximum deviation = 0.090 (1) Å], making dihedral angles of 9.55 (9)° in the complex with Pd1 and 7.28 (7)° in the complex with Pd2.

In the crystal structure, the K^+ ions interact with the various S and N atoms of the ligands with the distances of K···S = 3.6081 (13) Å and 3.6692 (13) Å, and K···N = 2.806 (3)–3.370 (5) Å, forming a three-dimensional polymeric network, and the short K···K contacts are present [4.4389 (17) Å and 4.4966 (18) Å]. Intra- and intramolecular C—H···S and C—H···N hydrogen bonds are also observed (Table 2).

Experimental

To a solution of Na_2PdCl_4 (0.1478 g, 0.502 mmol) in MeOH (30 ml) were added KSCN (0.5358 g, 5.513 mmol) and 2,2′-bipyrimidine (0.0819 g, 0.518 mmol), and refluxed for 3 h. The formed precipitate was separated by filtration and washed with H_2O and acetone, and dried at 50 °C, to give a pale red powder (0.1095 g). Red blocks were obtained by slow evaporation from a CH_3CN solution.

Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.95 Å with U_{iso}(H) = 1.2U_{eq}(C). The highest peak (0.65 e Å^{-3}) and the deepest hole (-0.59 e Å^{-3}) in the difference Fourier map are located 0.71 Å and 0.83 Å, respectively, from the Pd1 atom.

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

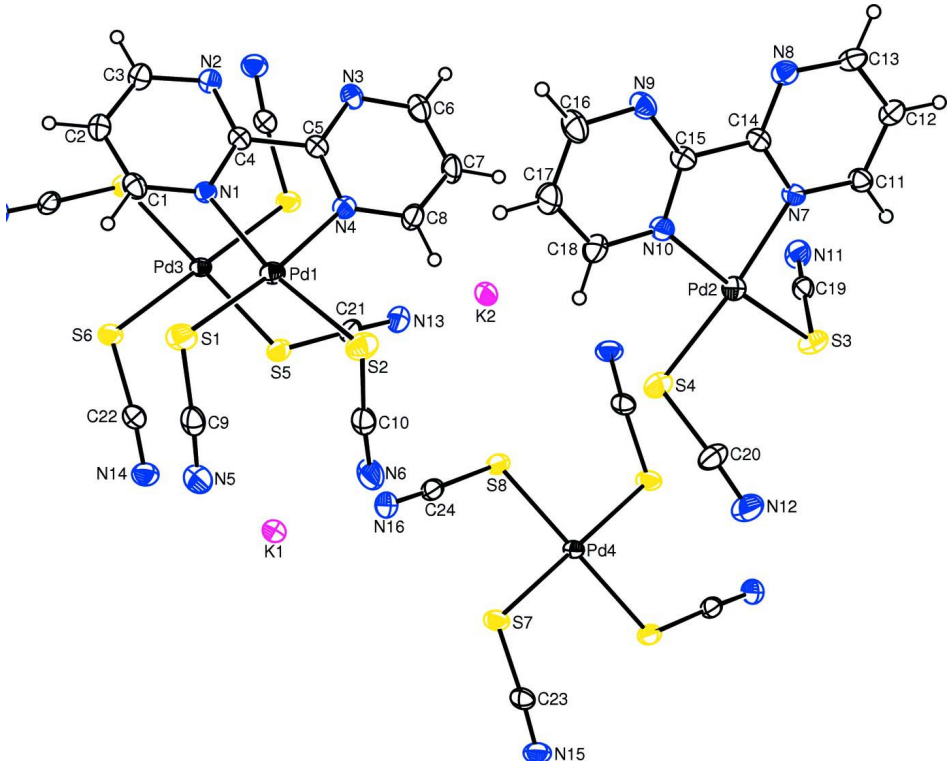

Figure 1

A structure detail of the title compound, with displacement ellipsoids drawn at the 30% probability level for non-H atoms. Unlabelled atoms are generated by the application of the inversion centres.

Dipotassium tetrakis(thiocyanato-κS)palladate(II)– (2,2′-bipyrimidine-$\kappa^2N^1,N^{1'}$)bis(thiocyanato- κS)palladium(II) (1/2)

Crystal data

$K_2[Pd(NCS)_4]\cdot 2[Pd(NCS)_2(C_8H_6N_4)]$
M_r = 1178.38
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 15.9625 (7) Å
b = 10.9700 (5) Å
c = 21.6801 (9) Å
β = 94.104 (1)°
V = 3786.6 (3) Å^3
Z = 4
F(000) = 2288
D_x = 2.067 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5010 reflections
θ = 2.5–26.0°
μ = 2.12 mm^{-1}

T = 200 K
Block, red

0.28 × 0.24 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.854, T_{max} = 1.000

22881 measured reflections
7371 independent reflections
5722 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°, θ_{min} = 1.3°
h = −18→19
k = −12→13
l = −25→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.08
7371 reflections
481 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
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 1.0988P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Special details

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

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Pd1	0.482313 (18)	0.51068 (2)	0.188694 (12)	0.03065 (9)
Pd2	−0.014348 (18)	−0.00967 (2)	−0.182524 (12)	0.02913 (8)
Pd3	0.5000	0.5000	0.0000	0.02538 (10)
Pd4	0.0000	1.0000	0.0000	0.02620 (10)
K1	0.42675 (5)	0.96456 (8)	0.08137 (4)	0.0397 (2)
K2	0.09465 (6)	0.52691 (8)	−0.07076 (4)	0.0426 (2)
S1	0.59836 (7)	0.62463 (10)	0.21959 (5)	0.0483 (3)
S2	0.39550 (7)	0.62960 (10)	0.24449 (5)	0.0498 (3)
S3	0.13902 (6)	0.40429 (9)	−0.28031 (5)	0.0412 (2)
S4	0.05796 (7)	−0.17773 (10)	−0.21091 (5)	0.0515 (3)
S5	0.41359 (6)	0.64489 (9)	0.04273 (5)	0.0376 (2)
S6	0.61598 (6)	0.62728 (9)	0.01879 (5)	0.0396 (2)
S7	0.11212 (6)	1.12966 (9)	0.02391 (5)	0.0448 (3)
S8	0.09601 (6)	0.84561 (9)	−0.01933 (5)	0.0405 (2)
N1	0.55052 (17)	0.3754 (2)	0.14802 (12)	0.0263 (6)

N2	0.53434 (18)	0.1777 (3)	0.10408 (12)	0.0312 (7)
N3	0.36456 (18)	0.1932 (3)	0.11846 (13)	0.0330 (7)
N4	0.38671 (18)	0.3913 (3)	0.16051 (12)	0.0302 (7)
N5	0.5592 (2)	0.8652 (3)	0.18054 (17)	0.0528 (9)
N6	0.3527 (2)	0.8499 (4)	0.18235 (19)	0.0607 (11)
N7	−0.06619 (17)	0.1506 (3)	−0.15385 (12)	0.0280 (6)
N8	−0.02642 (18)	0.3475 (3)	−0.11603 (13)	0.0347 (7)
N9	0.13917 (19)	0.2811 (3)	−0.12042 (14)	0.0381 (8)
N10	0.09353 (18)	0.0838 (3)	−0.15250 (13)	0.0320 (7)
N11	0.17991 (19)	0.5602 (3)	−0.17926 (16)	0.0460 (9)
N12	−0.0430 (3)	−0.3800 (4)	−0.1863 (2)	0.0694 (12)
N13	0.2462 (2)	0.5816 (3)	0.00536 (17)	0.0509 (9)
N14	0.5701 (2)	0.8743 (3)	0.02917 (15)	0.0427 (8)
N15	0.0555 (2)	1.3726 (3)	0.03105 (16)	0.0469 (9)
N16	0.2599 (2)	0.9214 (3)	0.02070 (17)	0.0516 (9)
C1	0.6330 (2)	0.3698 (4)	0.14158 (16)	0.0353 (9)
H1	0.6675	0.4368	0.1549	0.042*
C2	0.6693 (2)	0.2698 (3)	0.11627 (16)	0.0355 (9)
H2	0.7280	0.2661	0.1118	0.043*
C3	0.6171 (2)	0.1759 (4)	0.09784 (16)	0.0372 (9)
H3	0.6407	0.1062	0.0798	0.045*
C4	0.5048 (2)	0.2778 (3)	0.12903 (14)	0.0268 (8)
C5	0.4131 (2)	0.2861 (3)	0.13633 (14)	0.0272 (8)
C6	0.2825 (2)	0.2081 (4)	0.12340 (17)	0.0402 (10)
H6	0.2458	0.1427	0.1117	0.048*
C7	0.2488 (2)	0.3139 (4)	0.14461 (18)	0.0441 (10)
H7	0.1899	0.3243	0.1459	0.053*
C8	0.3038 (2)	0.4030 (4)	0.16362 (17)	0.0398 (9)
H8	0.2825	0.4764	0.1797	0.048*
C9	0.5728 (2)	0.7657 (4)	0.19553 (18)	0.0411 (10)
C10	0.3729 (2)	0.7573 (4)	0.20423 (18)	0.0405 (10)
C11	−0.1472 (2)	0.1804 (3)	−0.15213 (16)	0.0329 (8)
H11	−0.1894	0.1226	−0.1647	0.039*
C12	−0.1702 (2)	0.2942 (3)	−0.13225 (16)	0.0370 (9)
H12	−0.2277	0.3157	−0.1307	0.044*
C13	−0.1075 (2)	0.3756 (3)	−0.11476 (17)	0.0378 (9)
H13	−0.1225	0.4546	−0.1013	0.045*
C14	−0.0094 (2)	0.2372 (3)	−0.13530 (15)	0.0293 (8)
C15	0.0802 (2)	0.2000 (3)	−0.13587 (15)	0.0309 (8)
C16	0.2179 (2)	0.2413 (4)	−0.12183 (19)	0.0487 (11)
H16	0.2624	0.2973	−0.1126	0.058*
C17	0.2379 (3)	0.1234 (4)	−0.1360 (2)	0.0517 (11)
H17	0.2946	0.0969	−0.1352	0.062*
C18	0.1730 (2)	0.0461 (4)	−0.15129 (19)	0.0445 (10)
H18	0.1846	−0.0363	−0.1613	0.053*
C19	0.1617 (2)	0.4984 (3)	−0.22118 (18)	0.0342 (9)
C20	−0.0035 (3)	−0.2959 (4)	−0.19531 (18)	0.0452 (10)
C21	0.3143 (2)	0.6055 (3)	0.02093 (17)	0.0379 (9)
C22	0.5851 (2)	0.7726 (4)	0.02536 (16)	0.0328 (8)

C23	0.0761 (2)	1.2729 (4)	0.02831 (17)	0.0362 (9)
C24	0.1932 (2)	0.8932 (3)	0.00439 (17)	0.0373 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.03478 (17)	0.02747 (16)	0.02909 (15)	−0.00023 (12)	−0.00199 (12)	−0.00338 (12)
Pd2	0.03272 (16)	0.02533 (16)	0.02903 (15)	−0.00017 (12)	0.00016 (12)	−0.00167 (12)
Pd3	0.0290 (2)	0.0225 (2)	0.02406 (19)	0.00083 (15)	−0.00188 (15)	0.00014 (15)
Pd4	0.0283 (2)	0.0216 (2)	0.0280 (2)	−0.00027 (15)	−0.00313 (16)	0.00051 (16)
K1	0.0359 (5)	0.0320 (5)	0.0517 (5)	−0.0038 (4)	0.0055 (4)	−0.0031 (4)
K2	0.0389 (5)	0.0381 (5)	0.0512 (5)	−0.0072 (4)	0.0072 (4)	−0.0074 (4)
S1	0.0455 (6)	0.0389 (6)	0.0580 (7)	−0.0035 (5)	−0.0140 (5)	−0.0123 (5)
S2	0.0631 (7)	0.0439 (6)	0.0430 (6)	0.0079 (5)	0.0090 (5)	−0.0079 (5)
S3	0.0449 (6)	0.0334 (6)	0.0442 (6)	0.0121 (4)	−0.0041 (5)	−0.0023 (5)
S4	0.0507 (7)	0.0383 (6)	0.0668 (7)	0.0042 (5)	0.0134 (6)	−0.0161 (6)
S5	0.0363 (5)	0.0318 (5)	0.0449 (5)	0.0030 (4)	0.0035 (4)	−0.0079 (4)
S6	0.0338 (5)	0.0279 (5)	0.0558 (6)	−0.0010 (4)	−0.0051 (5)	−0.0041 (5)
S7	0.0336 (6)	0.0276 (5)	0.0713 (7)	−0.0023 (4)	−0.0106 (5)	−0.0040 (5)
S8	0.0338 (5)	0.0302 (5)	0.0568 (6)	0.0030 (4)	−0.0014 (5)	−0.0082 (5)
N1	0.0283 (16)	0.0246 (16)	0.0259 (14)	−0.0013 (12)	0.0002 (12)	−0.0035 (12)
N2	0.0306 (17)	0.0335 (18)	0.0294 (15)	−0.0005 (13)	0.0008 (13)	−0.0028 (14)
N3	0.0296 (17)	0.0369 (18)	0.0322 (16)	−0.0059 (14)	−0.0009 (13)	−0.0015 (14)
N4	0.0325 (17)	0.0305 (17)	0.0273 (15)	0.0023 (13)	0.0005 (13)	0.0041 (13)
N5	0.050 (2)	0.047 (2)	0.061 (2)	−0.0081 (19)	0.0080 (18)	−0.003 (2)
N6	0.035 (2)	0.054 (3)	0.092 (3)	−0.0003 (18)	−0.0020 (19)	0.028 (2)
N7	0.0288 (16)	0.0247 (16)	0.0302 (15)	−0.0014 (12)	−0.0001 (13)	0.0008 (13)
N8	0.0339 (18)	0.0308 (18)	0.0386 (17)	−0.0005 (14)	−0.0028 (14)	−0.0057 (14)
N9	0.0316 (18)	0.0382 (19)	0.0435 (18)	−0.0095 (15)	−0.0049 (14)	0.0035 (15)
N10	0.0316 (17)	0.0307 (18)	0.0333 (16)	−0.0012 (13)	0.0003 (13)	0.0021 (14)
N11	0.0307 (19)	0.051 (2)	0.055 (2)	0.0003 (16)	−0.0048 (16)	−0.0065 (19)
N12	0.079 (3)	0.041 (2)	0.092 (3)	0.017 (2)	0.035 (2)	0.011 (2)
N13	0.036 (2)	0.046 (2)	0.072 (2)	0.0018 (17)	0.0105 (18)	−0.0076 (19)
N14	0.046 (2)	0.034 (2)	0.0476 (19)	−0.0019 (16)	0.0009 (16)	−0.0057 (16)
N15	0.049 (2)	0.030 (2)	0.061 (2)	−0.0015 (16)	−0.0027 (17)	−0.0088 (17)
N16	0.032 (2)	0.045 (2)	0.078 (3)	0.0001 (16)	0.0049 (18)	−0.001 (2)
C1	0.031 (2)	0.040 (2)	0.034 (2)	−0.0060 (17)	−0.0021 (16)	0.0059 (17)
C2	0.030 (2)	0.042 (2)	0.034 (2)	0.0014 (17)	0.0050 (16)	0.0010 (18)
C3	0.033 (2)	0.042 (2)	0.037 (2)	0.0028 (18)	0.0042 (17)	−0.0032 (18)
C4	0.0296 (19)	0.030 (2)	0.0202 (17)	−0.0024 (15)	−0.0009 (14)	0.0026 (15)
C5	0.0303 (19)	0.030 (2)	0.0211 (17)	−0.0024 (16)	−0.0013 (14)	0.0025 (15)
C6	0.031 (2)	0.047 (3)	0.042 (2)	−0.0082 (18)	−0.0003 (17)	0.0030 (19)
C7	0.021 (2)	0.053 (3)	0.058 (3)	−0.0011 (18)	0.0021 (18)	0.006 (2)
C8	0.030 (2)	0.042 (2)	0.048 (2)	0.0082 (18)	0.0075 (18)	0.005 (2)
C9	0.034 (2)	0.050 (3)	0.040 (2)	−0.0090 (19)	0.0030 (17)	−0.014 (2)
C10	0.035 (2)	0.046 (3)	0.040 (2)	−0.0071 (19)	0.0047 (18)	−0.013 (2)
C11	0.031 (2)	0.031 (2)	0.037 (2)	−0.0038 (16)	0.0000 (16)	−0.0005 (17)
C12	0.035 (2)	0.036 (2)	0.039 (2)	0.0056 (17)	0.0010 (17)	−0.0055 (18)
C13	0.043 (2)	0.027 (2)	0.043 (2)	0.0051 (17)	−0.0013 (18)	−0.0066 (18)
C14	0.031 (2)	0.028 (2)	0.0278 (18)	−0.0038 (16)	0.0001 (15)	0.0011 (16)

C15	0.033 (2)	0.031 (2)	0.0280 (19)	−0.0020 (16)	−0.0033 (15)	0.0037 (16)
C16	0.032 (2)	0.058 (3)	0.055 (3)	−0.012 (2)	−0.0032 (19)	0.008 (2)
C17	0.029 (2)	0.054 (3)	0.071 (3)	0.002 (2)	0.000 (2)	0.009 (2)
C18	0.030 (2)	0.044 (2)	0.059 (3)	0.0055 (18)	0.0024 (19)	−0.002 (2)
C19	0.0235 (19)	0.035 (2)	0.044 (2)	0.0031 (16)	0.0012 (17)	0.0090 (19)
C20	0.059 (3)	0.039 (3)	0.039 (2)	0.017 (2)	0.013 (2)	0.001 (2)
C21	0.037 (2)	0.034 (2)	0.044 (2)	0.0084 (18)	0.0138 (19)	0.0008 (19)
C22	0.034 (2)	0.036 (2)	0.0283 (19)	−0.0049 (17)	−0.0007 (16)	−0.0011 (17)
C23	0.038 (2)	0.032 (2)	0.037 (2)	−0.0063 (17)	−0.0045 (17)	−0.0057 (18)
C24	0.040 (2)	0.031 (2)	0.042 (2)	0.0073 (18)	0.0102 (18)	0.0034 (18)

Geometric parameters (Å, º)

Pd1—N1	2.074 (3)	N3—C5	1.321 (4)
Pd1—N4	2.070 (3)	N3—C6	1.331 (4)
Pd1—S1	2.2945 (11)	N3—K1^{vi}	2.835 (3)
Pd1—S2	2.3077 (11)	N4—C8	1.336 (4)
Pd2—N7	2.059 (3)	N4—C5	1.348 (4)
Pd2—N10	2.069 (3)	N5—C9	1.155 (5)
Pd2—S3^{i}	2.2958 (10)	N6—C10	1.158 (5)
Pd2—S4	2.2829 (11)	N7—C11	1.337 (4)
Pd3—S5^{ii}	2.3388 (9)	N7—C14	1.354 (4)
Pd3—S5	2.3388 (9)	N8—C14	1.315 (4)
Pd3—S6^{ii}	2.3314 (9)	N8—C13	1.333 (4)
Pd3—S6	2.3314 (9)	N9—C15	1.321 (4)
Pd4—S7^{iii}	2.3157 (10)	N9—C16	1.333 (5)
Pd4—S7	2.3157 (10)	N10—C18	1.333 (5)
Pd4—S8^{iii}	2.3419 (10)	N10—C15	1.346 (4)
Pd4—S8	2.3419 (10)	N11—C19	1.154 (5)
K1—N14	2.806 (3)	N12—C20	1.142 (5)
K1—N3^{iv}	2.835 (3)	N12—K2^{vi}	3.370 (5)
K1—N6	2.853 (4)	N13—C21	1.146 (5)
K1—N2^{iv}	2.922 (3)	N14—C22	1.145 (5)
K1—N16	2.923 (4)	N14—K1^{v}	2.981 (3)
K1—N14^{v}	2.981 (3)	N15—C23	1.144 (5)
K1—N5	3.103 (4)	N15—K2^{iii}	2.827 (4)
K1—S5	3.6081 (13)	N15—K2^{iv}	2.886 (4)
K1—K1^{v}	4.4389 (17)	N16—C24	1.141 (5)
K2—N11	2.824 (4)	C1—C2	1.373 (5)
K2—N15^{iii}	2.827 (4)	C1—H1	0.9500
K2—N8	2.881 (3)	C2—C3	1.366 (5)
K2—N15^{vi}	2.886 (4)	C2—H2	0.9500
K2—N13	2.892 (4)	C3—H3	0.9500
K2—N9	3.008 (3)	C4—C5	1.486 (5)
K2—N12^{iv}	3.370 (5)	C6—C7	1.373 (5)
K2—S8	3.6692 (13)	C6—H6	0.9500
K2—K2^{vii}	4.4966 (18)	C7—C8	1.358 (5)
S1—C9	1.674 (5)	C7—H7	0.9500
S2—C10	1.676 (5)	C8—H8	0.9500
S3—C19	1.666 (4)	C11—C12	1.379 (5)

S3—Pd2^{viii}	2.2958 (10)	C11—H11	0.9500
S4—C20	1.675 (5)	C12—C13	1.375 (5)
S5—C21	1.677 (4)	C12—H12	0.9500
S6—C22	1.678 (4)	C13—H13	0.9500
S7—C23	1.679 (4)	C14—C15	1.487 (5)
S8—C24	1.683 (4)	C16—C17	1.372 (6)
N1—C1	1.336 (4)	C16—H16	0.9500
N1—C4	1.344 (4)	C17—C18	1.361 (6)
N2—C4	1.325 (4)	C17—H17	0.9500
N2—C3	1.338 (4)	C18—H18	0.9500
N2—K1^{vi}	2.922 (3)		

N4—Pd1—N1	79.65 (11)	C10—S2—Pd1	108.31 (14)
N4—Pd1—S1	173.55 (8)	C19—S3—Pd2^{viii}	98.67 (13)
N1—Pd1—S1	94.39 (8)	C20—S4—Pd2	104.84 (14)
N4—Pd1—S2	93.13 (8)	C21—S5—Pd3	106.57 (13)
N1—Pd1—S2	168.65 (8)	C21—S5—K1	110.74 (13)
S1—Pd1—S2	92.38 (4)	Pd3—S5—K1	136.58 (4)
N7—Pd2—N10	79.94 (11)	C22—S6—Pd3	110.44 (13)
N7—Pd2—S4	173.34 (8)	C23—S7—Pd4	108.97 (13)
N10—Pd2—S4	93.40 (9)	C24—S8—Pd4	108.78 (13)
N7—Pd2—S3^{i}	95.74 (8)	C24—S8—K2	111.96 (13)
N10—Pd2—S3^{i}	174.43 (8)	Pd4—S8—K2	138.91 (4)
S4—Pd2—S3^{i}	90.90 (4)	C1—N1—C4	116.7 (3)
S6^{ii}—Pd3—S6	180.00 (5)	C1—N1—Pd1	128.9 (2)
S6^{ii}—Pd3—S5^{ii}	90.42 (3)	C4—N1—Pd1	114.2 (2)
S6—Pd3—S5^{ii}	89.58 (3)	C4—N2—C3	115.8 (3)
S6^{ii}—Pd3—S5	89.58 (3)	C4—N2—K1^{vi}	120.7 (2)
S6—Pd3—S5	90.42 (3)	C3—N2—K1^{vi}	123.0 (2)
S5^{ii}—Pd3—S5	180.00 (6)	C5—N3—C6	116.2 (3)
S7^{iii}—Pd4—S7	180.00 (6)	C5—N3—K1^{vi}	123.7 (2)
S7^{iii}—Pd4—S8^{iii}	88.80 (3)	C6—N3—K1^{vi}	119.8 (2)
S7—Pd4—S8^{iii}	91.20 (3)	C8—N4—C5	116.1 (3)
S7^{iii}—Pd4—S8	91.20 (3)	C8—N4—Pd1	129.5 (3)
S7—Pd4—S8	88.80 (4)	C5—N4—Pd1	114.3 (2)
S8^{iii}—Pd4—S8	180.00 (5)	C9—N5—K1	129.2 (3)
N14—K1—N3^{iv}	137.64 (9)	C10—N6—K1	125.6 (3)
N14—K1—N6	123.28 (11)	C11—N7—C14	116.7 (3)
N3^{iv}—K1—N6	89.98 (10)	C11—N7—Pd2	128.9 (2)
N14—K1—N2^{iv}	82.17 (9)	C14—N7—Pd2	114.4 (2)
N3^{iv}—K1—N2^{iv}	57.16 (8)	C14—N8—C13	116.3 (3)
N6—K1—N2^{iv}	119.60 (10)	C14—N8—K2	126.0 (2)
N14—K1—N16	120.30 (10)	C13—N8—K2	117.6 (2)
N3^{iv}—K1—N16	86.83 (9)	C15—N9—C16	115.5 (3)
N6—K1—N16	81.96 (10)	C15—N9—K2	120.8 (2)
N2^{iv}—K1—N16	135.31 (10)	C16—N9—K2	123.3 (3)
N14—K1—N14^{v}	79.86 (10)	C18—N10—C15	117.2 (3)
N3^{iv}—K1—N14^{v}	74.32 (9)	C18—N10—Pd2	128.5 (3)
N6—K1—N14^{v}	155.48 (10)	C15—N10—Pd2	114.2 (2)

N2^{iv}—K1—N14^{v}	67.52 (8)	C19—N11—K2	118.1 (3)
N16—K1—N14^{v}	78.53 (10)	C20—N12—K2^{vi}	91.9 (3)
N14—K1—N5	67.69 (10)	C21—N13—K2	162.4 (3)
N3^{iv}—K1—N5	110.45 (9)	C22—N14—K1	123.6 (3)
N6—K1—N5	67.21 (10)	C22—N14—K1^{v}	120.3 (3)
N2^{iv}—K1—N5	78.54 (9)	K1—N14—K1^{v}	100.14 (10)
N16—K1—N5	143.95 (10)	C23—N15—K2^{iii}	129.9 (3)
N14^{v}—K1—N5	135.69 (9)	C23—N15—K2^{iv}	116.2 (3)
N14—K1—S5	66.36 (7)	K2^{iii}—N15—K2^{iv}	103.82 (11)
N3^{iv}—K1—S5	155.51 (7)	C24—N16—K1	169.6 (3)
N6—K1—S5	74.30 (9)	N1—C1—C2	121.7 (3)
N2^{iv}—K1—S5	147.20 (7)	N1—C1—H1	119.2
N16—K1—S5	72.67 (7)	C2—C1—H1	119.2
N14^{v}—K1—S5	113.18 (7)	C3—C2—C1	117.0 (3)
N5—K1—S5	81.08 (7)	C3—C2—H2	121.5
N14—K1—K1^{v}	41.39 (7)	C1—C2—H2	121.5
N3^{iv}—K1—K1^{v}	106.59 (7)	N2—C3—C2	123.0 (4)
N6—K1—K1^{v}	163.30 (9)	N2—C3—H3	118.5
N2^{iv}—K1—K1^{v}	69.94 (6)	C2—C3—H3	118.5
N16—K1—K1^{v}	100.68 (8)	N2—C4—N1	125.7 (3)
N14^{v}—K1—K1^{v}	38.47 (7)	N2—C4—C5	118.4 (3)
N5—K1—K1^{v}	103.93 (7)	N1—C4—C5	115.8 (3)
S5—K1—K1^{v}	90.63 (3)	N3—C5—N4	125.5 (3)
N11—K2—N15^{iii}	132.28 (10)	N3—C5—C4	118.9 (3)
N11—K2—N8	98.97 (9)	N4—C5—C4	115.6 (3)
N15^{iii}—K2—N8	78.92 (9)	N3—C6—C7	122.8 (4)
N11—K2—N15^{vi}	148.93 (10)	N3—C6—H6	118.6
N15^{iii}—K2—N15^{vi}	76.18 (11)	C7—C6—H6	118.6
N8—K2—N15^{vi}	71.51 (9)	C8—C7—C6	116.7 (4)
N11—K2—N13	90.88 (10)	C8—C7—H7	121.6
N15^{iii}—K2—N13	115.96 (10)	C6—C7—H7	121.6
N8—K2—N13	148.14 (10)	N4—C8—C7	122.5 (4)
N15^{vi}—K2—N13	84.46 (10)	N4—C8—H8	118.8
N11—K2—N9	71.18 (9)	C7—C8—H8	118.8
N15^{iii}—K2—N9	133.30 (9)	N5—C9—S1	176.3 (4)
N8—K2—N9	55.62 (8)	N6—C10—S2	172.0 (4)
N15^{vi}—K2—N9	79.48 (9)	N7—C11—C12	120.6 (3)
N13—K2—N9	100.43 (9)	N7—C11—H11	119.7
N11—K2—N12^{iv}	70.69 (9)	C12—C11—H11	119.7
N15^{iii}—K2—N12^{iv}	65.57 (10)	C13—C12—C11	118.0 (3)
N8—K2—N12^{iv}	64.42 (10)	C13—C12—H12	121.0
N15^{vi}—K2—N12^{iv}	125.51 (10)	C11—C12—H12	121.0
N13—K2—N12^{iv}	146.66 (11)	N8—C13—C12	122.2 (3)
N9—K2—N12^{iv}	99.44 (9)	N8—C13—H13	118.9
N11—K2—C19	16.81 (8)	C12—C13—H13	118.9
N15^{iii}—K2—C19	129.62 (9)	N8—C14—N7	126.1 (3)
N8—K2—C19	82.22 (9)	N8—C14—C15	118.4 (3)
N15^{vi}—K2—C19	138.92 (9)	N7—C14—C15	115.4 (3)
N13—K2—C19	104.47 (9)	N9—C15—N10	125.6 (3)

N9—K2—C19	59.54 (8)	N9—C15—C14	118.8 (3)
N12^{iv}—K2—C19	64.12 (9)	N10—C15—C14	115.6 (3)
N11—K2—S8	97.90 (8)	N9—C16—C17	123.2 (4)
N15^{iii}—K2—S8	61.49 (7)	N9—C16—H16	118.4
N8—K2—S8	138.05 (7)	C17—C16—H16	118.4
N15^{vi}—K2—S8	108.87 (7)	C18—C17—C16	117.2 (4)
N13—K2—S8	69.04 (7)	C18—C17—H17	121.4
N9—K2—S8	165.17 (7)	C16—C17—H17	121.4
N12^{iv}—K2—S8	85.78 (7)	N10—C18—C17	121.2 (4)
C19—K2—S8	111.77 (7)	N10—C18—H18	119.4
N11—K2—K2^{vii}	166.57 (8)	C17—C18—H18	119.4
N15^{iii}—K2—K2^{vii}	38.55 (7)	N11—C19—S3	177.2 (4)
N8—K2—K2^{vii}	71.07 (6)	N11—C19—K2	45.1 (2)
N15^{vi}—K2—K2^{vii}	37.63 (7)	S3—C19—K2	134.80 (17)
N13—K2—K2^{vii}	102.31 (8)	N12—C20—S4	176.7 (4)
N9—K2—K2^{vii}	108.30 (7)	N13—C21—S5	178.1 (4)
N12^{iv}—K2—K2^{vii}	96.47 (7)	N14—C22—S6	174.8 (4)
C19—K2—K2^{vii}	152.22 (7)	N15—C23—S7	176.6 (4)
S8—K2—K2^{vii}	84.69 (3)	N16—C24—S8	177.7 (4)
C9—S1—Pd1	103.83 (14)		

N1—Pd1—S1—C9	130.92 (16)	S4—Pd2—N10—C15	173.9 (2)
S2—Pd1—S1—C9	−58.20 (15)	N15^{iii}—K2—N11—C19	−88.3 (3)
N4—Pd1—S2—C10	−104.11 (16)	N8—K2—N11—C19	−5.2 (3)
N1—Pd1—S2—C10	−154.2 (4)	N15^{vi}—K2—N11—C19	63.7 (4)
S1—Pd1—S2—C10	79.23 (14)	N13—K2—N11—C19	144.4 (3)
N10—Pd2—S4—C20	145.08 (17)	N9—K2—N11—C19	43.7 (3)
S3^{i}—Pd2—S4—C20	−38.46 (16)	N12^{iv}—K2—N11—C19	−64.0 (3)
S6^{ii}—Pd3—S5—C21	−15.44 (14)	S8—K2—N11—C19	−146.6 (3)
S6—Pd3—S5—C21	164.56 (14)	K2^{vii}—K2—N11—C19	−46.4 (6)
S6^{ii}—Pd3—S5—K1	−163.85 (6)	N11—K2—N13—C21	−1.9 (10)
S6—Pd3—S5—K1	16.15 (6)	N15^{iii}—K2—N13—C21	−141.0 (10)
N14—K1—S5—C21	−147.04 (16)	N8—K2—N13—C21	106.8 (10)
N3^{iv}—K1—S5—C21	22.9 (2)	N15^{vi}—K2—N13—C21	147.3 (10)
N6—K1—S5—C21	74.78 (16)	N9—K2—N13—C21	69.1 (10)
N2^{iv}—K1—S5—C21	−164.47 (17)	N12^{iv}—K2—N13—C21	−56.5 (11)
N16—K1—S5—C21	−11.52 (16)	C19—K2—N13—C21	8.1 (11)
N14^{v}—K1—S5—C21	−80.41 (16)	S8—K2—N13—C21	−100.0 (10)
N5—K1—S5—C21	143.48 (16)	K2^{vii}—K2—N13—C21	−179.3 (10)
K1^{v}—K1—S5—C21	−112.52 (14)	N3^{iv}—K1—N14—C22	170.0 (3)
N14—K1—S5—Pd3	0.49 (9)	N6—K1—N14—C22	34.0 (4)
N3^{iv}—K1—S5—Pd3	170.47 (15)	N2^{iv}—K1—N14—C22	154.4 (3)
N6—K1—S5—Pd3	−137.68 (9)	N16—K1—N14—C22	−67.0 (4)
N2^{iv}—K1—S5—Pd3	−16.93 (14)	N14^{v}—K1—N14—C22	−137.2 (4)
N16—K1—S5—Pd3	136.02 (9)	N5—K1—N14—C22	73.6 (3)
N14^{v}—K1—S5—Pd3	67.13 (9)	S5—K1—N14—C22	−16.2 (3)
N5—K1—S5—Pd3	−68.98 (9)	K1^{v}—K1—N14—C22	−137.2 (4)
K1^{v}—K1—S5—Pd3	35.02 (6)	N3^{iv}—K1—N14—K1^{v}	−52.87 (16)
S5^{ii}—Pd3—S6—C22	157.74 (14)	N6—K1—N14—K1^{v}	171.15 (11)

S5—Pd3—S6—C22	−22.26 (14)	N2^{iv}—K1—N14—K1^{v}	−68.44 (9)
S8—Pd4—S7—C23	168.18 (15)	N16—K1—N14—K1^{v}	70.22 (13)
S7^{iii}—Pd4—S8—C24	−170.46 (14)	N14^{v}—K1—N14—K1^{v}	0.0
S7—Pd4—S8—C24	9.54 (14)	N5—K1—N14—K1^{v}	−149.21 (12)
S7^{iii}—Pd4—S8—K2	1.77 (7)	S5—K1—N14—K1^{v}	120.99 (9)
S7—Pd4—S8—K2	−178.23 (7)	N14—K1—N16—C24	110.1 (18)
N11—K2—S8—C24	−69.23 (16)	N3^{iv}—K1—N16—C24	−104.3 (18)
N15^{iii}—K2—S8—C24	156.54 (17)	N6—K1—N16—C24	−13.9 (18)
N8—K2—S8—C24	177.82 (17)	N2^{iv}—K1—N16—C24	−138.4 (17)
N15^{vi}—K2—S8—C24	94.77 (16)	N5—K1—N16—C24	16.9 (19)
N13—K2—S8—C24	18.67 (16)	S5—K1—N16—C24	62.1 (18)
N9—K2—S8—C24	−27.7 (3)	K1^{v}—K1—N16—C24	149.4 (18)
N12^{iv}—K2—S8—C24	−139.05 (16)	C4—N1—C1—C2	0.6 (5)
C19—K2—S8—C24	−79.09 (16)	Pd1—N1—C1—C2	176.4 (2)
K2^{vii}—K2—S8—C24	124.04 (14)	N1—C1—C2—C3	0.0 (5)
N11—K2—S8—Pd4	118.71 (9)	C4—N2—C3—C2	0.6 (5)
N15^{iii}—K2—S8—Pd4	−15.52 (10)	K1^{vi}—N2—C3—C2	−170.9 (3)
N8—K2—S8—Pd4	5.76 (13)	C1—C2—C3—N2	−0.7 (5)
N15^{vi}—K2—S8—Pd4	−77.29 (10)	C3—N2—C4—N1	0.1 (5)
N13—K2—S8—Pd4	−153.39 (10)	K1^{vi}—N2—C4—N1	171.9 (2)
N9—K2—S8—Pd4	160.2 (2)	C3—N2—C4—C5	179.1 (3)
N12^{iv}—K2—S8—Pd4	48.89 (9)	K1^{vi}—N2—C4—C5	−9.1 (4)
C19—K2—S8—Pd4	108.84 (9)	C1—N1—C4—N2	−0.7 (5)
K2^{vii}—K2—S8—Pd4	−48.03 (7)	Pd1—N1—C4—N2	−177.1 (3)
N4—Pd1—N1—C1	179.1 (3)	C1—N1—C4—C5	−179.7 (3)
S1—Pd1—N1—C1	−3.3 (3)	Pd1—N1—C4—C5	3.9 (4)
S2—Pd1—N1—C1	−129.7 (4)	C6—N3—C5—N4	2.2 (5)
N4—Pd1—N1—C4	−5.0 (2)	K1^{vi}—N3—C5—N4	−172.4 (2)
S1—Pd1—N1—C4	172.5 (2)	C6—N3—C5—C4	−176.9 (3)
S2—Pd1—N1—C4	46.1 (5)	K1^{vi}—N3—C5—C4	8.5 (4)
N1—Pd1—N4—C8	−175.6 (3)	C8—N4—C5—N3	−3.3 (5)
S2—Pd1—N4—C8	13.3 (3)	Pd1—N4—C5—N3	175.9 (3)
N1—Pd1—N4—C5	5.4 (2)	C8—N4—C5—C4	175.9 (3)
S2—Pd1—N4—C5	−165.8 (2)	Pd1—N4—C5—C4	−5.0 (3)
N14—K1—N5—C9	−80.2 (4)	N2—C4—C5—N3	0.8 (5)
N3^{iv}—K1—N5—C9	145.5 (4)	N1—C4—C5—N3	179.9 (3)
N6—K1—N5—C9	64.5 (4)	N2—C4—C5—N4	−178.4 (3)
N2^{iv}—K1—N5—C9	−166.3 (4)	N1—C4—C5—N4	0.7 (4)
N16—K1—N5—C9	31.1 (5)	C5—N3—C6—C7	1.2 (5)
N14^{v}—K1—N5—C9	−126.3 (4)	K1^{vi}—N3—C6—C7	176.0 (3)
S5—K1—N5—C9	−12.2 (4)	N3—C6—C7—C8	−3.1 (6)
K1^{v}—K1—N5—C9	−100.6 (4)	C5—N4—C8—C7	1.0 (5)
N14—K1—N6—C10	−6.0 (4)	Pd1—N4—C8—C7	−178.0 (3)
N3^{iv}—K1—N6—C10	−158.1 (4)	C6—C7—C8—N4	1.9 (6)
N2^{iv}—K1—N6—C10	−106.7 (4)	C14—N7—C11—C12	0.0 (5)
N16—K1—N6—C10	115.1 (4)	Pd2—N7—C11—C12	−178.9 (3)
N14^{v}—K1—N6—C10	152.6 (3)	N7—C11—C12—C13	0.4 (5)
N5—K1—N6—C10	−45.8 (4)	C14—N8—C13—C12	0.3 (5)
S5—K1—N6—C10	41.0 (4)	K2—N8—C13—C12	−176.5 (3)

K1^{v}—K1—N6—C10	14.7 (6)	C11—C12—C13—N8	−0.6 (6)
N10—Pd2—N7—C11	−176.4 (3)	C13—N8—C14—N7	0.1 (5)
S3^{i}—Pd2—N7—C11	7.2 (3)	K2—N8—C14—N7	176.7 (2)
N10—Pd2—N7—C14	4.7 (2)	C13—N8—C14—C15	−178.3 (3)
S3^{i}—Pd2—N7—C14	−171.7 (2)	K2—N8—C14—C15	−1.7 (4)
N11—K2—N8—C14	63.2 (3)	C11—N7—C14—N8	−0.3 (5)
N15^{iii}—K2—N8—C14	−165.3 (3)	Pd2—N7—C14—N8	178.8 (3)
N15^{vi}—K2—N8—C14	−86.3 (3)	C11—N7—C14—C15	178.2 (3)
N13—K2—N8—C14	−43.3 (4)	Pd2—N7—C14—C15	−2.8 (4)
N9—K2—N8—C14	3.4 (3)	C16—N9—C15—N10	−0.1 (5)
N12^{iv}—K2—N8—C14	126.6 (3)	K2—N9—C15—N10	−172.9 (2)
C19—K2—N8—C14	61.7 (3)	C16—N9—C15—C14	179.8 (3)
S8—K2—N8—C14	175.7 (2)	K2—N9—C15—C14	7.1 (4)
K2^{vii}—K2—N8—C14	−126.1 (3)	C18—N10—C15—N9	2.4 (5)
N11—K2—N8—C13	−120.3 (3)	Pd2—N10—C15—N9	−173.7 (3)
N15^{iii}—K2—N8—C13	11.2 (3)	C18—N10—C15—C14	−177.6 (3)
N15^{vi}—K2—N8—C13	90.2 (3)	Pd2—N10—C15—C14	6.4 (4)
N13—K2—N8—C13	133.2 (3)	N8—C14—C15—N9	−3.8 (5)
N9—K2—N8—C13	180.0 (3)	N7—C14—C15—N9	177.7 (3)
N12^{iv}—K2—N8—C13	−56.8 (3)	N8—C14—C15—N10	176.1 (3)
C19—K2—N8—C13	−121.8 (3)	N7—C14—C15—N10	−2.4 (4)
S8—K2—N8—C13	−7.7 (3)	C15—N9—C16—C17	−2.3 (6)
K2^{vii}—K2—N8—C13	50.4 (2)	K2—N9—C16—C17	170.3 (3)
N11—K2—N9—C15	−121.0 (3)	N9—C16—C17—C18	2.3 (7)
N15^{iii}—K2—N9—C15	10.0 (3)	C15—N10—C18—C17	−2.3 (6)
N8—K2—N9—C15	−5.3 (2)	Pd2—N10—C18—C17	173.1 (3)
N15^{vi}—K2—N9—C15	69.4 (3)	C16—C17—C18—N10	0.1 (6)
N13—K2—N9—C15	151.7 (3)	Pd2^{viii}—S3—C19—K2	79.2 (2)
N12^{iv}—K2—N9—C15	−55.2 (3)	N15^{iii}—K2—C19—N11	106.2 (3)
C19—K2—N9—C15	−107.6 (3)	N8—K2—C19—N11	174.8 (3)
S8—K2—N9—C15	−164.9 (2)	N15^{vi}—K2—C19—N11	−135.2 (3)
K2^{vii}—K2—N9—C15	44.9 (3)	N13—K2—C19—N11	−36.9 (3)
N11—K2—N9—C16	66.8 (3)	N9—K2—C19—N11	−130.7 (3)
N15^{iii}—K2—N9—C16	−162.2 (3)	N12^{iv}—K2—C19—N11	109.5 (3)
N8—K2—N9—C16	−177.5 (3)	S8—K2—C19—N11	35.9 (3)
N15^{vi}—K2—N9—C16	−102.8 (3)	K2^{vii}—K2—C19—N11	158.9 (3)
N13—K2—N9—C16	−20.5 (3)	N11—K2—C19—S3	176.0 (5)
N12^{iv}—K2—N9—C16	132.6 (3)	N15^{iii}—K2—C19—S3	−77.8 (3)
C19—K2—N9—C16	80.2 (3)	N8—K2—C19—S3	−9.2 (2)
S8—K2—N9—C16	22.9 (5)	N15^{vi}—K2—C19—S3	40.8 (3)
K2^{vii}—K2—N9—C16	−127.3 (3)	N13—K2—C19—S3	139.1 (2)
N7—Pd2—N10—C18	178.4 (3)	N9—K2—C19—S3	45.3 (2)
S4—Pd2—N10—C18	−1.6 (3)	N12^{iv}—K2—C19—S3	−74.5 (2)
N7—Pd2—N10—C15	−6.1 (2)	S8—K2—C19—S3	−148.1 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···S1	0.95	2.77	3.334 (4)	119
C1—H1···N11^{ii}	0.95	2.45	3.134 (5)	128
C6—H6···S7^{vi}	0.95	2.76	3.457 (4)	131
C8—H8···S2	0.95	2.77	3.321 (4)	118
C11—H11···S3^{i}	0.95	2.82	3.371 (4)	118
C11—H11···N6^{vii}	0.95	2.63	3.315 (5)	130
C13—H13···N15^{iii}	0.95	2.61	3.376 (5)	138
C16—H16···S6^{ii}	0.95	2.83	3.640 (4)	144
C18—H18···S4	0.95	2.71	3.276 (4)	119

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