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Dibromido(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')(dimethyl sulfoxide-κO)-cadmium

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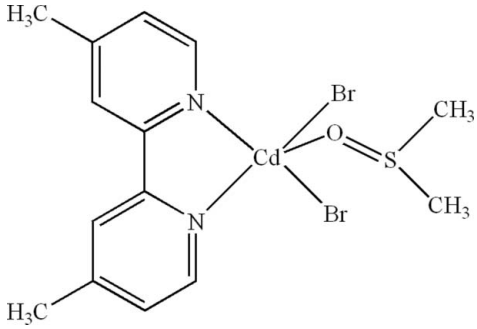
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.086; data-to-parameter ratio = 21.3.

In the title compound, $[CdBr_2(C_{12}H_{12}N_2)(C_2H_6OS)]$, the Cd^{II} atom is five-coordinated in a distorted trigonal–bipyramidal geometry by two N atoms from one 4,4′-dimethyl-2,2′-bipyridine (DMBP) ligand, one O atom from a dimethyl sulfoxide (DMSO) ligand and two Br atoms. A weak intramolecular C—H···O hydrogen bond occurs between the DMBP and DMSO ligands. π–π stacking between pyridine rings [centroid–centroid distances = 3.682 (3) and 3.598 (3) Å] is observed in the crystal.

Related literature

For related structures, see: Ahmadi *et al.* (2008); Alizadeh *et al.* (2010); Amani *et al.* (2009); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Sakamoto *et al.* (2004); Shirvan & Haydari Dezfuli (2011); Sofetis *et al.* (2006); Willett *et al.* (2001); Yoshikawa *et al.* (2003); Yousefi *et al.* (2008).



Experimental

Crystal data

$[CdBr_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
M_r = 534.58
Monoclinic, $P2_1/c$
a = 8.3940 (6) Å
b = 15.2928 (15) Å
c = 14.8606 (9) Å
β = 103.377 (5)°
V = 1855.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.59 mm^{-1}
T = 298 K
0.33 × 0.28 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.183, T_{max} = 0.342
16741 measured reflections
4054 independent reflections
3008 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.086
S = 1.04
4054 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1	2.301 (4)	Cd1—Br1	2.5857 (6)
Cd1—N1	2.349 (3)	Cd1—Br2	2.5784 (6)
Cd1—N2	2.340 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1	0.93	2.51	3.087 (5)	120

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: XU5571).

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supplementary materials

Acta Cryst. (2012). E**68**, m1006–m1007 [doi:10.1107/S1600536812028553]

Dibromido(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')(dimethyl sulfoxide-κO)cadmium

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Comment

4,4′-Dimethyl-2,2′-bipyridine (4,4′-dmbipy), is a good bidentate ligand, and numerous complexes with 4,4′-dmbipy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platin (Hojjat Kashani *et al.*, 2008), manganese (Sakamoto *et al.*, 2004), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), iridium (Yoshikawa *et al.*, 2003), cadmium (Kalateh *et al.*, 2010) and zinc (Alizadeh *et al.*, 2010; Shirvan & Haydari Dezfuli, 2011). Here, we report the synthesis and structure of the title compound.

In the title compound, (Fig. 1), the Cd^{II} atom is five-coordinated in a distorted trigonal-bipyramidal configuration by two N atoms from one 4,4′-dimethyl-2,2′-bipyridine, one O atom from one dimethyl sulfoxide and two Br atoms. The Cd—Br and Cd—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 2) and π-π contacts (Fig. 2) between the pyridine rings, *Cg*3—*Cg*2^{i} and *Cg*3—*Cg*3^{ii} [symmetry cods: (i) –*X*,-Y,1-*Z* and (ii) 1-*X*,-Y,1-*Z*, where *Cg*2 and *Cg*3 are centroids of the rings (N1/C1—C3/C5—C6) and (N2/C7—C9/C11—C12), respectively] may stabilize the structure, with centroid-centroid distance of 3.682 (3) and 3.598 (3) Å.

Experimental

For the preparation of the title compound, a solution of 4,4′-dimethyl-2,2′-bipyridine (0.25 g, 1.33 mmol) in methanol (10 ml) was added to a solution of $CdBr_2.4H_2O$, (0.46 g, 1.33 mmol) in methanol (10 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by methanol diffusion to a colorless solution in DMSO. Suitable crystals were isolated after one week (yield; 0.52 g, 73.1%).

Refinement

H atoms were positioned geometrically with C—H = 0.93–0.96 Å and constrained to ride on their parent atoms, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for the others.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

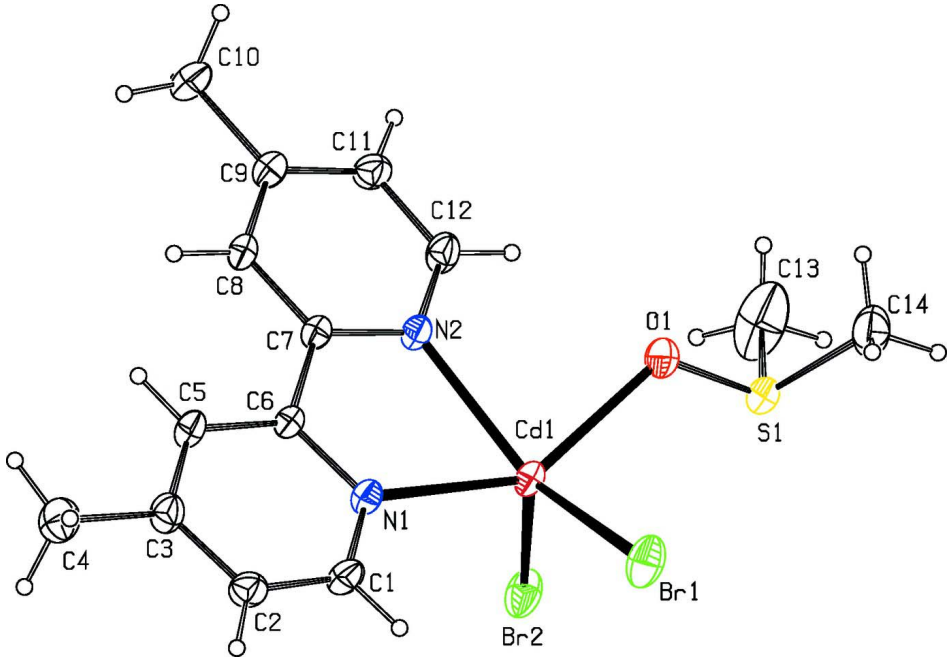

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

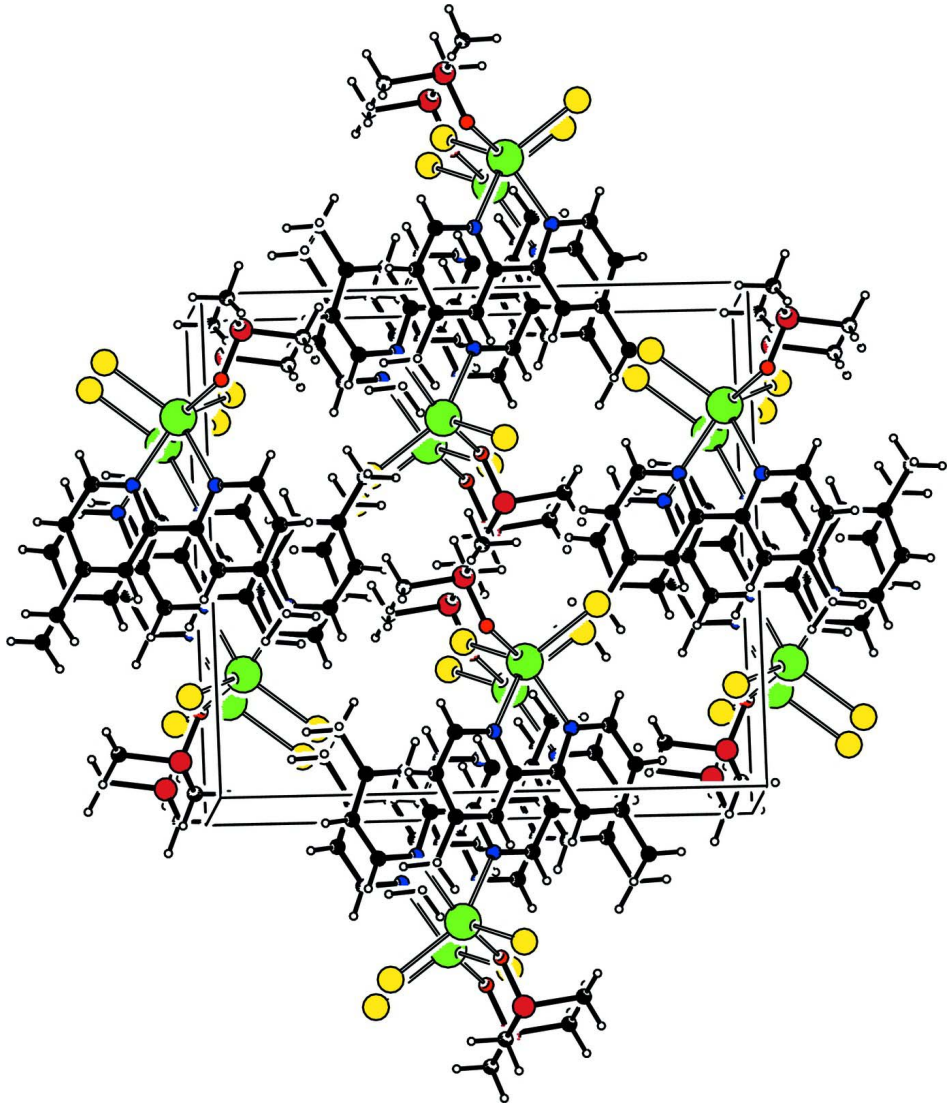

Figure 2

Unit-cell packing diagram for title compound.

Dibromido(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')(dimethyl sulfoxide-κO)cadmium

Crystal data

$[CdBr_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
$M_r = 534.58$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.3940\ (6)$ Å
$b = 15.2928\ (15)$ Å
$c = 14.8606\ (9)$ Å
$\beta = 103.377\ (5)°$
$V = 1855.9\ (3)$ Å^3
$Z = 4$
$F(000) = 1032$
$D_x = 1.913$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10741 reflections
$\theta = 1.9–27.0°$
$\mu = 5.59$ mm^{-1}
$T = 298$ K
Block, colorless
0.33 × 0.28 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.183, T_{max} = 0.342
16741 measured reflections
4054 independent reflections
3008 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
θ_{max} = 27.0°, θ_{min} = 1.9°
h = −9→10
k = −19→19
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.086
S = 1.04
4054 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2 + 0.8746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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}
C1	0.0502 (6)	0.2148 (3)	0.6246 (3)	0.0501 (11)
H1	0.0521	0.2350	0.6838	0.060*
C2	−0.0370 (7)	0.2624 (3)	0.5505 (3)	0.0526 (12)
H2	−0.0933	0.3127	0.5599	0.063*
C3	−0.0391 (7)	0.2337 (3)	0.4611 (3)	0.0528 (12)
C4	−0.1294 (8)	0.2827 (4)	0.3769 (4)	0.0767 (18)
H4A	−0.0862	0.3409	0.3779	0.092*
H4B	−0.2437	0.2854	0.3769	0.092*
H4C	−0.1160	0.2529	0.3223	0.092*
C5	0.0474 (6)	0.1592 (3)	0.4529 (3)	0.0473 (11)
H5	0.0502	0.1387	0.3944	0.057*
C6	0.1305 (5)	0.1138 (2)	0.5302 (2)	0.0373 (9)
C7	0.2243 (5)	0.0322 (2)	0.5237 (3)	0.0365 (9)
C8	0.2297 (6)	−0.0049 (3)	0.4393 (3)	0.0426 (10)
H8	0.1732	0.0214	0.3848	0.051*
C9	0.3177 (6)	−0.0803 (3)	0.4350 (3)	0.0476 (11)
C10	0.3268 (7)	−0.1202 (3)	0.3438 (3)	0.0634 (14)

H10A	0.2846	−0.1787	0.3402	0.076*
H10B	0.4387	−0.1213	0.3387	0.076*
H10C	0.2629	−0.0858	0.2943	0.076*
C11	0.3983 (7)	−0.1162 (3)	0.5174 (3)	0.0535 (12)
H11	0.4593	−0.1670	0.5178	0.064*
C12	0.3894 (7)	−0.0776 (3)	0.5995 (3)	0.0539 (12)
H12	0.4446	−0.1034	0.6545	0.065*
C13	0.5760 (15)	−0.1667 (4)	0.8786 (5)	0.144 (4)
H13A	0.6672	−0.1729	0.8502	0.173*
H13B	0.4795	−0.1906	0.8385	0.173*
H13C	0.5987	−0.1973	0.9365	0.173*
C14	0.7460 (8)	−0.0254 (5)	0.9509 (4)	0.094 (2)
H14A	0.7545	0.0372	0.9532	0.112*
H14B	0.8195	−0.0483	0.9159	0.112*
H14C	0.7744	−0.0485	1.0126	0.112*
N1	0.1310 (5)	0.1425 (2)	0.6162 (2)	0.0418 (8)
N2	0.3045 (5)	−0.0041 (2)	0.6035 (2)	0.0424 (8)
Br1	0.35504 (9)	0.19185 (4)	0.84879 (4)	0.0779 (2)
Br2	0.07055 (8)	−0.04712 (4)	0.79461 (3)	0.06865 (18)
O1	0.5107 (5)	−0.0161 (3)	0.8016 (2)	0.0663 (10)
S1	0.54455 (17)	−0.05549 (9)	0.89770 (7)	0.0547 (3)
Cd1	0.27102 (4)	0.05814 (2)	0.741841 (19)	0.04315 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.065 (3)	0.048 (2)	0.040 (2)	0.002 (2)	0.017 (2)	−0.0086 (18)
C2	0.060 (3)	0.046 (2)	0.053 (3)	0.011 (2)	0.016 (2)	−0.002 (2)
C3	0.062 (3)	0.051 (3)	0.043 (2)	0.005 (2)	0.007 (2)	0.0069 (19)
C4	0.094 (5)	0.076 (4)	0.058 (3)	0.032 (3)	0.014 (3)	0.017 (3)
C5	0.060 (3)	0.051 (2)	0.030 (2)	0.000 (2)	0.0084 (19)	0.0015 (17)
C6	0.043 (2)	0.040 (2)	0.0296 (19)	−0.0028 (18)	0.0094 (17)	−0.0016 (15)
C7	0.042 (2)	0.0367 (19)	0.0315 (18)	−0.0094 (17)	0.0090 (17)	−0.0005 (14)
C8	0.049 (3)	0.048 (2)	0.0295 (19)	−0.003 (2)	0.0061 (18)	0.0004 (16)
C9	0.057 (3)	0.047 (2)	0.039 (2)	−0.004 (2)	0.012 (2)	−0.0054 (17)
C10	0.083 (4)	0.067 (3)	0.045 (3)	0.001 (3)	0.024 (3)	−0.011 (2)
C11	0.062 (3)	0.050 (3)	0.051 (3)	0.012 (2)	0.017 (2)	−0.003 (2)
C12	0.069 (3)	0.050 (3)	0.039 (2)	0.009 (2)	0.006 (2)	0.0047 (18)
C13	0.262 (13)	0.059 (4)	0.091 (5)	0.014 (6)	0.003 (7)	0.010 (3)
C14	0.075 (5)	0.144 (6)	0.055 (3)	−0.019 (4)	0.001 (3)	0.000 (4)
N1	0.050 (2)	0.0409 (18)	0.0332 (17)	−0.0013 (17)	0.0076 (16)	−0.0039 (14)
N2	0.050 (2)	0.0457 (19)	0.0309 (16)	0.0009 (17)	0.0077 (15)	0.0003 (14)
Br1	0.1001 (5)	0.0708 (3)	0.0542 (3)	−0.0152 (3)	0.0004 (3)	−0.0206 (2)
Br2	0.0777 (4)	0.0856 (4)	0.0417 (3)	−0.0271 (3)	0.0118 (2)	0.0113 (2)
O1	0.066 (2)	0.091 (2)	0.0404 (17)	0.022 (2)	0.0083 (16)	0.0151 (17)
S1	0.0557 (7)	0.0726 (7)	0.0358 (5)	0.0043 (7)	0.0102 (5)	0.0008 (5)
Cd1	0.0511 (2)	0.04968 (17)	0.02831 (14)	−0.00105 (16)	0.00838 (12)	0.00028 (12)

Geometric parameters (Å, º)

C1—N1	1.318 (6)	C10—H10B	0.9600
C1—C2	1.380 (7)	C10—H10C	0.9600
C1—H1	0.9300	C11—C12	1.372 (6)
C2—C3	1.394 (6)	C11—H11	0.9300
C2—H2	0.9300	C12—N2	1.339 (6)
C3—C5	1.373 (7)	C12—H12	0.9300
C3—C4	1.504 (7)	C13—S1	1.754 (7)
C4—H4A	0.9600	C13—H13A	0.9600
C4—H4B	0.9600	C13—H13B	0.9600
C4—H4C	0.9600	C13—H13C	0.9600
C5—C6	1.384 (6)	C14—S1	1.755 (6)
C5—H5	0.9300	C14—H14A	0.9600
C6—N1	1.351 (5)	C14—H14B	0.9600
C6—C7	1.489 (6)	C14—H14C	0.9600
C7—N2	1.342 (5)	Cd1—O1	2.301 (4)
C7—C8	1.387 (5)	Cd1—N1	2.349 (3)
C8—C9	1.378 (6)	Cd1—N2	2.340 (3)
C8—H8	0.9300	Cd1—Br1	2.5857 (6)
C9—C11	1.370 (6)	Cd1—Br2	2.5784 (6)
C9—C10	1.505 (6)	O1—S1	1.515 (3)
C10—H10A	0.9600		
N1—C1—C2	123.8 (4)	C9—C11—H11	119.8
N1—C1—H1	118.1	C12—C11—H11	119.8
C2—C1—H1	118.1	N2—C12—C11	122.7 (4)
C1—C2—C3	118.8 (4)	N2—C12—H12	118.7
C1—C2—H2	120.6	C11—C12—H12	118.7
C3—C2—H2	120.6	S1—C13—H13A	109.5
C5—C3—C2	117.1 (4)	S1—C13—H13B	109.5
C5—C3—C4	121.0 (4)	H13A—C13—H13B	109.5
C2—C3—C4	121.9 (5)	S1—C13—H13C	109.5
C3—C4—H4A	109.5	H13A—C13—H13C	109.5
C3—C4—H4B	109.5	H13B—C13—H13C	109.5
H4A—C4—H4B	109.5	S1—C14—H14A	109.5
C3—C4—H4C	109.5	S1—C14—H14B	109.5
H4A—C4—H4C	109.5	H14A—C14—H14B	109.5
H4B—C4—H4C	109.5	S1—C14—H14C	109.5
C3—C5—C6	121.2 (4)	H14A—C14—H14C	109.5
C3—C5—H5	119.4	H14B—C14—H14C	109.5
C6—C5—H5	119.4	C1—N1—C6	118.3 (4)
N1—C6—C5	120.8 (4)	C1—N1—Cd1	124.0 (3)
N1—C6—C7	116.6 (3)	C6—N1—Cd1	117.7 (3)
C5—C6—C7	122.6 (3)	C12—N2—C7	118.1 (3)
N2—C7—C8	121.0 (4)	C12—N2—Cd1	123.6 (3)
N2—C7—C6	117.0 (3)	C7—N2—Cd1	118.1 (3)
C8—C7—C6	122.0 (4)	S1—O1—Cd1	121.1 (2)
C9—C8—C7	120.9 (4)	O1—S1—C13	103.6 (3)
C9—C8—H8	119.5	O1—S1—C14	105.7 (3)

C7—C8—H8	119.5	C13—S1—C14	99.3 (5)
C11—C9—C8	116.9 (4)	O1—Cd1—N2	82.34 (12)
C11—C9—C10	121.7 (4)	O1—Cd1—N1	144.06 (13)
C8—C9—C10	121.3 (4)	N2—Cd1—N1	70.41 (12)
C9—C10—H10A	109.5	O1—Cd1—Br2	98.54 (10)
C9—C10—H10B	109.5	N2—Cd1—Br2	103.45 (9)
H10A—C10—H10B	109.5	N1—Cd1—Br2	110.05 (9)
C9—C10—H10C	109.5	O1—Cd1—Br1	93.61 (10)
H10A—C10—H10C	109.5	N2—Cd1—Br1	142.22 (9)
H10B—C10—H10C	109.5	N1—Cd1—Br1	93.99 (8)
C9—C11—C12	120.3 (4)	Br2—Cd1—Br1	114.28 (2)
N1—C1—C2—C3	−0.9 (8)	C8—C7—N2—C12	−0.3 (6)
C1—C2—C3—C5	−0.2 (7)	C6—C7—N2—C12	179.9 (4)
C1—C2—C3—C4	−179.2 (5)	C8—C7—N2—Cd1	−175.5 (3)
C2—C3—C5—C6	1.1 (7)	C6—C7—N2—Cd1	4.6 (5)
C4—C3—C5—C6	−179.9 (5)	Cd1—O1—S1—C13	122.3 (5)
C3—C5—C6—N1	−1.0 (7)	Cd1—O1—S1—C14	−133.7 (3)
C3—C5—C6—C7	179.4 (4)	S1—O1—Cd1—N2	−145.6 (3)
N1—C6—C7—N2	−1.8 (6)	S1—O1—Cd1—N1	174.01 (19)
C5—C6—C7—N2	177.7 (4)	S1—O1—Cd1—Br2	−43.1 (3)
N1—C6—C7—C8	178.4 (4)	S1—O1—Cd1—Br1	72.1 (3)
C5—C6—C7—C8	−2.1 (6)	C12—N2—Cd1—O1	24.8 (4)
N2—C7—C8—C9	0.0 (7)	C7—N2—Cd1—O1	−160.3 (3)
C6—C7—C8—C9	179.8 (4)	C12—N2—Cd1—N1	−179.0 (4)
C7—C8—C9—C11	0.1 (7)	C7—N2—Cd1—N1	−4.1 (3)
C7—C8—C9—C10	−178.9 (5)	C12—N2—Cd1—Br2	−72.2 (4)
C8—C9—C11—C12	0.1 (8)	C7—N2—Cd1—Br2	102.7 (3)
C10—C9—C11—C12	179.1 (5)	C12—N2—Cd1—Br1	110.8 (4)
C9—C11—C12—N2	−0.4 (8)	C7—N2—Cd1—Br1	−74.3 (4)
C2—C1—N1—C6	1.0 (7)	C1—N1—Cd1—O1	−135.5 (4)
C2—C1—N1—Cd1	−177.5 (4)	C6—N1—Cd1—O1	46.0 (4)
C5—C6—N1—C1	0.0 (6)	C1—N1—Cd1—N2	−178.5 (4)
C7—C6—N1—C1	179.5 (4)	C6—N1—Cd1—N2	3.1 (3)
C5—C6—N1—Cd1	178.5 (3)	C1—N1—Cd1—Br2	83.9 (4)
C7—C6—N1—Cd1	−1.9 (5)	C6—N1—Cd1—Br2	−94.6 (3)
C11—C12—N2—C7	0.5 (7)	C1—N1—Cd1—Br1	−33.8 (4)
C11—C12—N2—Cd1	175.5 (4)	C6—N1—Cd1—Br1	147.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1	0.93	2.51	3.087 (5)	120