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(4,4′-Dimethyl-2,2′-bipyridine-κ^2N,N')-(dimethyl sulfoxide-κO)diiodidocadmium(II)

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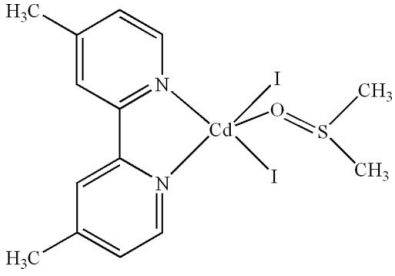
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.066; wR factor = 0.172; data-to-parameter ratio = 27.5.

In the title compound, $[CdI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$, the Cd^{II} cation is coordinated by two N atoms from a dimethylbipyridine ligand, one O atom from a dimethyl sulfoxide molecule and two I^- anions in a distorted trigonal–bipyramidal geometry. Intramolecular C—H···O hydrogen bonding and intermolecular π–π stacking between parallel pyridine rings [centroid–centroid distance = 3.658 (3) Å] are present in the crystal structure.

Related literature

For metal complexes of 4,4′-dimethyl-2,2′-bipyridine, see: Ahmadi *et al.* (2008); Amani *et al.* (2009); Kalateh *et al.* (2008); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Sakamoto *et al.* (2004); Sofetis *et al.* (2006); Willett *et al.* (2001); Yoshikawa *et al.* (2003); Yousefi *et al.* (2008).



Experimental

Crystal data

$[CdI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
M_r = 628.58
Monoclinic, $P2_1/c$
a = 8.729 (1) Å
b = 15.5247 (18) Å
c = 15.1354 (17) Å
β = 102.620 (9)°
V = 2001.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.28 mm^{-1}
T = 298 K
0.49 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.002, T_{max} = 0.055
15568 measured reflections
5360 independent reflections
4625 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.172
S = 1.16
5360 reflections
195 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.10 e Å^{-3}
$\Delta\rho_{min}$ = −2.23 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.366 (5)	Cd1—I1	2.7535 (6)
Cd1—N2	2.326 (4)	Cd1—I2	2.7674 (6)
Cd1—O1	2.313 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1	0.93	2.47	3.063 (8)	122

Data collection: *SMART* (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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2734).

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supporting information

Acta Cryst. (2010). E**66**, m512 [https://doi.org/10.1107/S1600536810012572]

(4,4′-Dimethyl-2,2′-bipyridine-κ^2N,N')(dimethyl sulfoxide-κO)diiodidocadmium(II)

Khadijeh Kalateh, Roya Ahmadi and Vahid Amani

S1. 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) and iridium (Yoshikawa *et al.*, 2003). 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 square-pyramidal configuration by two N atoms from one 4,4′-dimethyl-2,2′-bipyridine, one O atom from one dimethyl sulfoxide and two I atoms. The Cd—I 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, Cg3—$Cg2^{i}$ and Cg3—$Cg3^{ii}$ [symmetry cods: (i) 2-X,2-Y,2-Z and (ii) 1-X,2-Y,2-Z , where Cg2 and Cg3 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 3.657 (3) and 3.775 (3) Å.

S2. Experimental

For the preparation of the title compound a solution of 4,4′-dimethyl-2,2′-bipyridine (0.15 g, 0.80 mmol) in methanol (10 ml) was added to a solution of CdI_2 (0.29 g, 0.80 mmol) in methanol (5 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; 0.36 g, 71.6%).

S3. Refinement

All H atoms were positioned geometrically with C—H = 0.93 (aromatic) and 0.96 Å (methyl) and constrained to ride on their parent atoms, with $U_{iso}(H)=1.2U_{eq}(c)$.

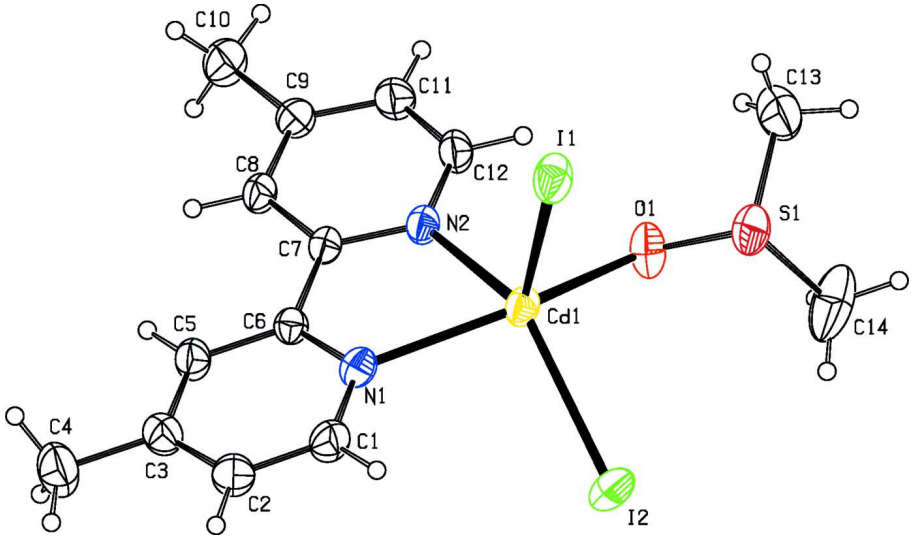

Figure 1

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

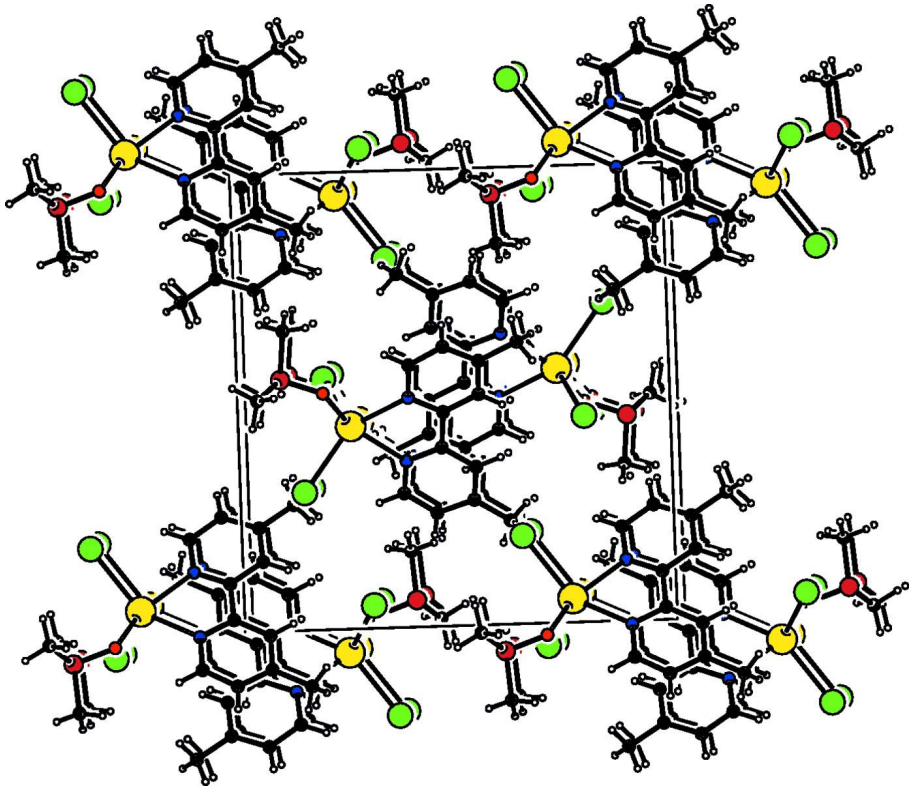

Figure 2

Unit-cell packing diagram for (I).

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Crystal data

$[CdI_2(C_{12}H_{12}N_2)(C_2H_6OS)]$
$M_r = 628.58$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.729$ (1) Å
$b = 15.5247$ (18) Å
$c = 15.1354$ (17) Å
$\beta = 102.620$ (9)°
$V = 2001.5$ (4) Å^3
$Z = 4$
$F(000) = 1176$
$D_x = 2.086$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 887 reflections
$\theta = 1.9$–$29.3°$
$\mu = 4.28$ mm^{-1}
$T = 298$ K
Block, colorless
0.49 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.002$, $T_{max} = 0.055$
15568 measured reflections
5360 independent reflections
4625 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 29.2°$, $\theta_{min} = 1.9°$
$h = -11 \rightarrow 11$
$k = -21 \rightarrow 20$
$l = -20 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.172$
$S = 1.16$
5360 reflections
195 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
$w = 1/[\sigma^2(F_o^2) + (0.0903P)^2 + 1.8883P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.015$
$\Delta\rho_{max} = 2.10$ e Å^{-3}
$\Delta\rho_{min} = -2.23$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0171 (10)

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.9509 (8)	0.7934 (4)	0.8795 (4)	0.0575 (14)
H1	0.9529	0.7743	0.8216	0.069*
C2	1.0322 (8)	0.7476 (4)	0.9527 (5)	0.0596 (14)

H2	1.0897	0.6991	0.9439	0.071*
C3	1.0280 (8)	0.7741 (4)	1.0397 (4)	0.0584 (14)
C4	1.1139 (11)	0.7258 (6)	1.1206 (6)	0.082 (2)
H4C	1.1322	0.7630	1.1725	0.098*
H4B	1.2126	0.7060	1.1101	0.098*
H4A	1.0522	0.6773	1.1313	0.098*
C5	0.9435 (7)	0.8469 (4)	1.0476 (4)	0.0499 (12)
H5	0.9383	0.8666	1.1049	0.060*
C6	0.8651 (5)	0.8918 (3)	0.9714 (3)	0.0385 (9)
C7	0.7726 (5)	0.9709 (3)	0.9790 (3)	0.0385 (9)
C8	0.7692 (6)	1.0072 (4)	1.0620 (3)	0.0453 (10)
H8	0.8262	0.9825	1.1151	0.054*
C9	0.6794 (7)	1.0810 (4)	1.0656 (4)	0.0488 (11)
C10	0.6735 (10)	1.1201 (5)	1.1561 (4)	0.0679 (17)
H10A	0.7188	1.1767	1.1603	0.081*
H10B	0.7315	1.0846	1.2037	0.081*
H10C	0.5663	1.1239	1.1617	0.081*
C11	0.5989 (8)	1.1146 (4)	0.9857 (4)	0.0568 (13)
H11	0.5372	1.1635	0.9857	0.068*
C12	0.6086 (8)	1.0764 (4)	0.9054 (4)	0.0545 (13)
H12	0.5546	1.1013	0.8517	0.065*
C13	0.411 (3)	1.1614 (9)	0.6212 (9)	0.189 (11)
H13A	0.3652	1.1675	0.6730	0.227*
H13B	0.3365	1.1789	0.5677	0.227*
H13C	0.5029	1.1971	0.6287	0.227*
C14	0.2811 (10)	1.0103 (11)	0.5584 (6)	0.110 (4)
H14C	0.2942	0.9510	0.5437	0.132*
H14B	0.2383	1.0418	0.5040	0.132*
H14A	0.2108	1.0141	0.5989	0.132*
N1	0.8687 (5)	0.8647 (3)	0.8888 (3)	0.0471 (9)
N2	0.6925 (5)	1.0048 (3)	0.9006 (3)	0.0439 (9)
O1	0.4994 (6)	1.0216 (4)	0.7072 (3)	0.0664 (12)
Cd1	0.72703 (5)	0.94561 (3)	0.76515 (2)	0.04529 (16)
I1	0.93442 (5)	1.04931 (3)	0.70096 (3)	0.06676 (19)
I2	0.63195 (7)	0.80423 (3)	0.65550 (3)	0.0758 (2)
S1	0.46338 (19)	1.05399 (12)	0.61041 (10)	0.0574 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.068 (3)	0.057 (3)	0.046 (3)	0.009 (3)	0.008 (2)	−0.013 (2)
C2	0.066 (3)	0.056 (3)	0.055 (3)	0.014 (3)	0.010 (3)	−0.008 (3)
C3	0.062 (3)	0.055 (3)	0.056 (3)	0.010 (3)	0.007 (3)	0.003 (3)
C4	0.094 (5)	0.082 (5)	0.063 (4)	0.032 (4)	0.006 (4)	0.008 (4)
C5	0.055 (3)	0.054 (3)	0.038 (2)	0.008 (2)	0.005 (2)	0.000 (2)
C6	0.038 (2)	0.042 (2)	0.036 (2)	−0.0003 (16)	0.0086 (16)	0.0007 (18)
C7	0.037 (2)	0.045 (2)	0.033 (2)	−0.0025 (17)	0.0059 (16)	−0.0002 (18)
C8	0.054 (3)	0.050 (3)	0.031 (2)	0.003 (2)	0.0069 (18)	−0.0019 (19)

C9	0.055 (3)	0.048 (3)	0.045 (3)	0.002 (2)	0.013 (2)	−0.003 (2)
C10	0.090 (5)	0.070 (4)	0.046 (3)	0.011 (4)	0.019 (3)	−0.009 (3)
C11	0.068 (3)	0.051 (3)	0.050 (3)	0.013 (3)	0.010 (3)	−0.004 (2)
C12	0.069 (3)	0.055 (3)	0.036 (2)	0.014 (3)	0.002 (2)	0.002 (2)
C13	0.38 (3)	0.084 (8)	0.079 (7)	0.051 (13)	−0.012 (12)	0.009 (6)
C14	0.061 (4)	0.200 (13)	0.063 (5)	−0.027 (6)	0.001 (4)	−0.007 (7)
N1	0.050 (2)	0.053 (2)	0.038 (2)	−0.0004 (18)	0.0086 (17)	−0.0057 (18)
N2	0.048 (2)	0.048 (2)	0.0333 (18)	0.0019 (17)	0.0039 (16)	−0.0008 (17)
O1	0.059 (2)	0.095 (4)	0.042 (2)	0.014 (2)	0.0060 (18)	0.010 (2)
Cd1	0.0492 (2)	0.0532 (3)	0.0323 (2)	−0.00441 (14)	0.00650 (14)	−0.00210 (14)
I1	0.0659 (3)	0.0866 (4)	0.0452 (2)	−0.0248 (2)	0.00653 (18)	0.01257 (19)
I2	0.0940 (4)	0.0675 (3)	0.0581 (3)	−0.0181 (2)	−0.0001 (2)	−0.0193 (2)
S1	0.0532 (7)	0.0810 (11)	0.0364 (6)	0.0013 (6)	0.0061 (5)	−0.0011 (6)

Geometric parameters (Å, º)

C1—N1	1.342 (8)	C10—H10B	0.9600
C1—C2	1.376 (9)	C10—H10C	0.9600
C1—H1	0.9300	C11—C12	1.373 (8)
C2—C3	1.387 (9)	C11—H11	0.9300
C2—H2	0.9300	C12—N2	1.342 (8)
C3—C5	1.368 (8)	C12—H12	0.9300
C3—C4	1.491 (9)	C13—S1	1.746 (13)
C4—H4C	0.9600	C13—H13A	0.9600
C4—H4B	0.9600	C13—H13B	0.9600
C4—H4A	0.9600	C13—H13C	0.9600
C5—C6	1.393 (7)	C14—S1	1.751 (9)
C5—H5	0.9300	C14—H14C	0.9600
C6—N1	1.327 (6)	C14—H14B	0.9600
C6—C7	1.487 (7)	C14—H14A	0.9600
C7—N2	1.346 (6)	Cd1—N1	2.366 (5)
C7—C8	1.384 (7)	Cd1—N2	2.326 (4)
C8—C9	1.396 (8)	O1—S1	1.515 (5)
C8—H8	0.9300	Cd1—O1	2.313 (5)
C9—C11	1.363 (9)	Cd1—I1	2.7535 (6)
C9—C10	1.508 (8)	Cd1—I2	2.7674 (6)
C10—H10A	0.9600		

N1—C1—C2	122.4 (6)	C9—C11—H11	120.0
N1—C1—H1	118.8	C12—C11—H11	120.0
C2—C1—H1	118.8	N2—C12—C11	123.1 (5)
C1—C2—C3	119.6 (6)	N2—C12—H12	118.5
C1—C2—H2	120.2	C11—C12—H12	118.5
C3—C2—H2	120.2	S1—C13—H13A	109.5
C5—C3—C2	117.0 (6)	S1—C13—H13B	109.5
C5—C3—C4	121.8 (6)	H13A—C13—H13B	109.5
C2—C3—C4	121.1 (6)	S1—C13—H13C	109.5
C3—C4—H4C	109.5	H13A—C13—H13C	109.5

C3—C4—H4B	109.5	H13B—C13—H13C	109.5
H4C—C4—H4B	109.5	S1—C14—H14C	109.5
C3—C4—H4A	109.5	S1—C14—H14B	109.5
H4C—C4—H4A	109.5	H14C—C14—H14B	109.5
H4B—C4—H4A	109.5	S1—C14—H14A	109.5
C3—C5—C6	121.2 (5)	H14C—C14—H14A	109.5
C3—C5—H5	119.4	H14B—C14—H14A	109.5
C6—C5—H5	119.4	C6—N1—C1	118.9 (5)
N1—C6—C5	120.9 (5)	C6—N1—Cd1	117.5 (4)
N1—C6—C7	117.4 (4)	C1—N1—Cd1	123.6 (4)
C5—C6—C7	121.8 (4)	C12—N2—C7	117.5 (5)
N2—C7—C8	122.1 (5)	C12—N2—Cd1	123.5 (3)
N2—C7—C6	116.2 (4)	C7—N2—Cd1	118.7 (3)
C8—C7—C6	121.7 (4)	S1—O1—Cd1	121.0 (3)
C7—C8—C9	119.6 (5)	O1—Cd1—N2	82.36 (16)
C7—C8—H8	120.2	O1—Cd1—N1	145.92 (16)
C9—C8—H8	120.2	N2—Cd1—N1	70.02 (16)
C11—C9—C8	117.7 (5)	O1—Cd1—I1	98.31 (14)
C11—C9—C10	122.5 (6)	N2—Cd1—I1	107.57 (12)
C8—C9—C10	119.8 (5)	N1—Cd1—I1	108.61 (12)
C9—C10—H10A	109.5	O1—Cd1—I2	93.25 (14)
C9—C10—H10B	109.5	N2—Cd1—I2	139.68 (12)
H10A—C10—H10B	109.5	N1—Cd1—I2	95.15 (12)
C9—C10—H10C	109.5	I1—Cd1—I2	112.72 (2)
H10A—C10—H10C	109.5	O1—S1—C13	103.3 (5)
H10B—C10—H10C	109.5	O1—S1—C14	106.4 (5)
C9—C11—C12	120.0 (6)	C13—S1—C14	100.5 (9)

N1—C1—C2—C3	1.3 (11)	C8—C7—N2—C12	0.5 (8)
C1—C2—C3—C5	−1.2 (11)	C6—C7—N2—C12	−179.7 (5)
C1—C2—C3—C4	179.6 (8)	C8—C7—N2—Cd1	174.2 (4)
C2—C3—C5—C6	0.2 (10)	C6—C7—N2—Cd1	−6.0 (6)
C4—C3—C5—C6	179.4 (7)	S1—O1—Cd1—N2	152.1 (4)
C3—C5—C6—N1	0.8 (9)	S1—O1—Cd1—N1	−172.4 (3)
C3—C5—C6—C7	179.9 (6)	S1—O1—Cd1—I1	45.3 (4)
N1—C6—C7—N2	4.0 (7)	S1—O1—Cd1—I2	−68.2 (4)
C5—C6—C7—N2	−175.1 (5)	C12—N2—Cd1—O1	−22.7 (5)
N1—C6—C7—C8	−176.1 (5)	C7—N2—Cd1—O1	164.0 (4)
C5—C6—C7—C8	4.8 (8)	C12—N2—Cd1—N1	177.6 (5)
N2—C7—C8—C9	0.4 (8)	C7—N2—Cd1—N1	4.3 (4)
C6—C7—C8—C9	−179.4 (5)	C12—N2—Cd1—I1	73.7 (5)
C7—C8—C9—C11	−0.4 (9)	C7—N2—Cd1—I1	−99.6 (4)
C7—C8—C9—C10	179.2 (6)	C12—N2—Cd1—I2	−108.7 (5)
C8—C9—C11—C12	−0.5 (10)	C7—N2—Cd1—I2	78.0 (4)
C10—C9—C11—C12	180.0 (7)	C6—N1—Cd1—O1	−39.9 (6)
C9—C11—C12—N2	1.5 (11)	C1—N1—Cd1—O1	139.8 (5)
C5—C6—N1—C1	−0.8 (8)	C6—N1—Cd1—N2	−2.0 (4)
C7—C6—N1—C1	−179.9 (5)	C1—N1—Cd1—N2	177.7 (5)

C5—C6—N1—Cd1	179.0 (4)	C6—N1—Cd1—I1	100.5 (4)
C7—C6—N1—Cd1	−0.2 (6)	C1—N1—Cd1—I1	−79.8 (5)
C2—C1—N1—C6	−0.3 (10)	C6—N1—Cd1—I2	−143.5 (4)
C2—C1—N1—Cd1	−180.0 (5)	C1—N1—Cd1—I2	36.2 (5)
C11—C12—N2—C7	−1.4 (10)	Cd1—O1—S1—C13	−131.6 (9)
C11—C12—N2—Cd1	−174.8 (5)	Cd1—O1—S1—C14	123.1 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1	0.93	2.47	3.063 (8)	122