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catena-Poly[[(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')cadmium]-di-μ-bromido]

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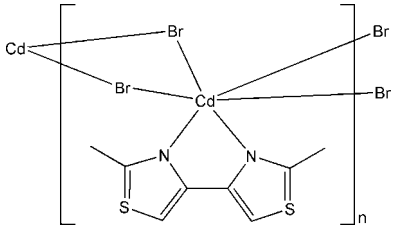
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; R factor = 0.081; wR factor = 0.232; data-to-parameter ratio = 25.0.

In the title coordination polymer, $[CdBr_2(C_8H_8N_2S_2)]_n$, the Cd^{II} atom is six-coordinated in a distorted octahedral geometry by two N atoms from a 2,2′-dimethyl-4,4′-bi-1,3-thiazole ligand and four bridging Br atoms. The bridging function of the Br atoms leads to a chain structure along [100]. Interchain C—H···Br hydrogen bonds and π–π contacts between the thiazole rings [centroid–centroid distances = 3.810 (5) and 3.679 (5) Å] are observed.

Related literature

For metal complexes with 2,2′-dimethyl-4,4′-bi-1,3-thiazole, see: Abedi (2011); Abedi & Yahyazade Bali (2010); Al-Hashemi *et al.* (2009, 2010); Khavasi *et al.* (2008); Notash *et al.* (2008, 2009); Safari *et al.* (2009).



Experimental

Crystal data

$[CdBr_2(C_8H_8N_2S_2)]$
M_r = 468.51
Triclinic, $P\overline{1}$
a = 7.1936 (10) Å
b = 9.5775 (11) Å
c = 10.4218 (14) Å
α = 112.714 (9)°
β = 104.149 (11)°
γ = 92.68 (1)°
V = 634.20 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.32 mm^{-1}
T = 298 K
0.28 × 0.18 × 0.13 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.180, T_{max} = 0.340
7003 measured reflections
3400 independent reflections
2495 reflections with $I > 2\sigma(I)$
R_{int} = 0.160

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.232
S = 1.05
3400 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.22 e Å^{-3}
$\Delta\rho_{min}$ = −4.78 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.435 (7)	Cd1—Br2^{i}	2.7640 (12)
Cd1—N2	2.372 (7)	Cd1—Br1^{ii}	2.8362 (12)
Cd1—Br1	2.7112 (11)	Cd1—Br2	2.7845 (12)

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···Br1^{iii}	0.93	2.87	3.754 (11)	159
C6—H6···Br1^{iii}	0.93	2.86	3.772 (10)	166
C8—H8*C*···Br2	0.96	2.74	3.681 (16)	167

Symmetry code: (iii) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (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: HY2437).

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supporting information

Acta Cryst. (2011). E**67**, m886 [doi:10.1107/S1600536811020861]

catena-Poly[[(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')cadmium]-di-μ-bromido]

Anita Abedi and Forugh Rezaei

S1. Comment

Recently, we reported the synthesis and crystal structures of [HgI_2(dm4bt)] (Abedi & Yahyazade Bali, 2010) and [$HgBr_2$(dm4bt)] (Abedi, 2011) (dm4bt = 2,2′-dimethyl-4,4′-bi-1,3-thiazole). Dm4bt is a good bidentate ligand, and numerous complexes with dm4bt have been prepared, such as that of zinc (Khavasi *et al.*, 2008), thallium (Notash *et al.*, 2008), cadmium (Notash *et al.*, 2009), mercury (Safari *et al.*, 2009) and copper (Al-Hashemi *et al.*, 2009, 2010). For further investigation of dm4bt, we synthesized the title complex and report herein its crystal structure.

In the title coordination polymer (Fig. 1), the Cd^{II} atom is six-coordinated in a distorted octahedral geometry by two N atoms from a dm4bt ligand and four bridging Br atoms (Table 1). The bridging function of the bromide atoms leads to a one-dimensional chain structure along [1 0 0] (Fig. 2).

In the crystal structure, intermolecular C—H···Br hydrogen bonds (Table 2) and π–π contacts (Fig. 2) between the thiazole rings, *Cg*4···*Cg*5^{i} = 3.810 (5) and *Cg*5···*Cg*5^{ii} = 3.679 (5) Å [symmetry codes: (i) 1-x, 2-y, 1-z; (ii) -x, 2-y, 1-z. *Cg*4 and *Cg*5 are the centroids of the S1/C2/N1/C4/C3 and S2/C6/C5/N2/C7 rings], stabilize the structure.

S2. Experimental

For the preparation of the title compound, a solution of dm4bt (0.26 g, 1.3 mmol) in methanol (15 ml) was added to a solution of $CdBr_2.4H_2O$ (0.44 g, 1.3 mmol) in methanol (15 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by methanol diffusion into a colorless solution in DMF. The crystals were isolated after one week (yield: 0.45 g, 73.9%).

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (CH) and 0.96 (CH_3) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C). The highest residual electron density was found at 0.89 Å from Cd1 atom and the deepest hole at 0.88 Å from Cd1 atom.

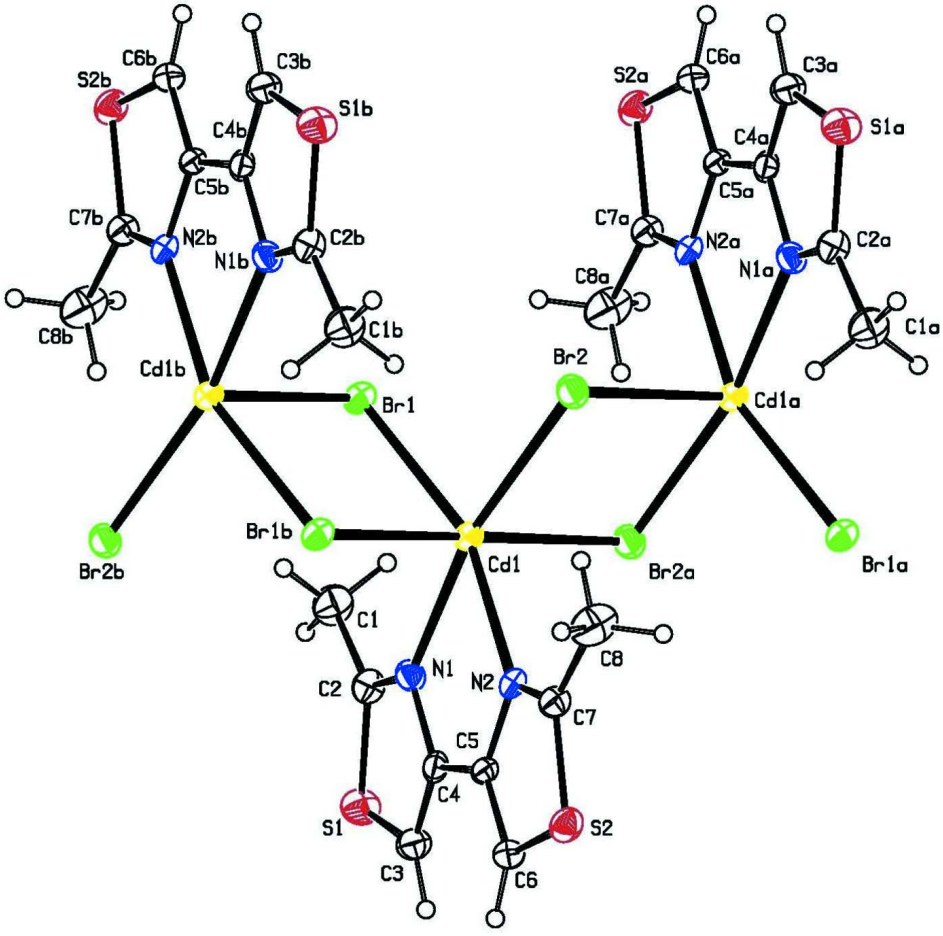

Figure 1

Part of the chain structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (a) -x, 1-y, 1-z; (b) 1-x, 1-y, 1-z.]

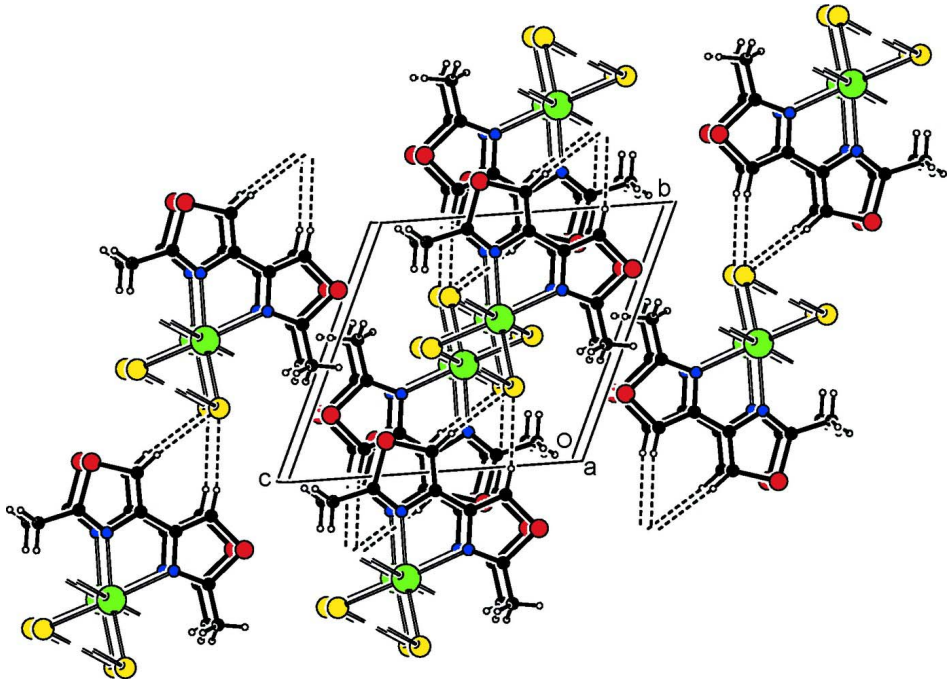

Figure 2

The packing diagram for the title compound.

catena-Poly[[(2,2′-dimethyl-4,4′-bi-1,3-thiazole-κ^2N,N')cadmium]-di-μ-bromido]

Crystal data

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$b = 9.5775\ (11)$ Å
$c = 10.4218\ (14)$ Å
$\alpha = 112.714\ (9)°$
$\beta = 104.149\ (11)°$
$\gamma = 92.68\ (1)°$
$V = 634.20\ (16)$ Å^3
$Z = 2$
$F(000) = 440$
$D_x = 2.454$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7003 reflections
$\theta = 2.2–29.2°$
$\mu = 8.32$ mm^{-1}
$T = 298$ K
Block, colorless
0.28 × 0.18 × 0.13 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.180$, $T_{max} = 0.340$
7003 measured reflections
3400 independent reflections
2495 reflections with $I > 2\sigma(I)$
$R_{int} = 0.160$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.2°$
$h = -9\rightarrow9$
$k = -13\rightarrow12$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.081$
$wR(F^2) = 0.232$
$S = 1.05$
3400 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.149P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 2.22$ e Å^{-3}
$\Delta\rho_{min} = -4.78$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2848 (18)	0.4579 (13)	0.0750 (12)	0.050 (3)
H1A	0.1742	0.3946	0.0710	0.060*
H1B	0.4015	0.4317	0.1221	0.060*
H1C	0.2854	0.4415	−0.0218	0.060*
C2	0.2745 (13)	0.6214 (11)	0.1579 (9)	0.0338 (18)
C3	0.2515 (14)	0.8908 (11)	0.2347 (10)	0.0362 (19)
H3	0.2437	0.9918	0.2478	0.043*
C4	0.2597 (11)	0.8389 (10)	0.3383 (9)	0.0277 (16)
C5	0.2502 (11)	0.9274 (9)	0.4849 (9)	0.0262 (15)
C6	0.2499 (13)	1.0824 (10)	0.5464 (10)	0.0342 (18)
H6	0.2571	1.1478	0.5004	0.041*
C7	0.2327 (13)	0.9521 (11)	0.7021 (10)	0.0332 (18)
C8	0.220 (2)	0.9124 (16)	0.8265 (12)	0.057 (3)
H8C	0.2207	0.8045	0.7987	0.068*
H8B	0.1028	0.9388	0.8511	0.068*
H8A	0.3300	0.9686	0.9089	0.068*
N1	0.2720 (11)	0.6838 (9)	0.2955 (8)	0.0298 (14)
N2	0.2379 (10)	0.8540 (8)	0.5760 (8)	0.0282 (14)
Cd1	0.24677 (9)	0.58678 (7)	0.47579 (7)	0.0302 (2)
Br1	0.36362 (13)	0.31498 (11)	0.34631 (11)	0.0364 (3)
Br2	0.14395 (13)	0.49070 (11)	0.67291 (10)	0.0353 (3)
S1	0.2574 (4)	0.7476 (3)	0.0763 (2)	0.0420 (6)
S2	0.2347 (4)	1.1375 (3)	0.7182 (2)	0.0364 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.056 (6)	0.038 (5)	0.047 (6)	0.009 (5)	0.019 (5)	0.007 (4)
C2	0.034 (4)	0.035 (5)	0.030 (4)	0.007 (4)	0.009 (3)	0.011 (3)
C3	0.041 (5)	0.032 (5)	0.038 (4)	0.009 (4)	0.013 (4)	0.016 (4)
C4	0.023 (4)	0.033 (4)	0.031 (4)	0.010 (3)	0.012 (3)	0.014 (3)
C5	0.022 (4)	0.021 (4)	0.036 (4)	0.005 (3)	0.008 (3)	0.012 (3)
C6	0.035 (5)	0.026 (4)	0.045 (5)	0.007 (3)	0.016 (4)	0.016 (4)
C7	0.032 (4)	0.030 (4)	0.039 (4)	0.007 (3)	0.011 (3)	0.014 (4)

C8	0.084 (9)	0.059 (7)	0.037 (5)	0.032 (7)	0.026 (5)	0.021 (5)
N1	0.031 (4)	0.031 (4)	0.031 (3)	0.004 (3)	0.013 (3)	0.013 (3)
N2	0.025 (3)	0.028 (3)	0.035 (3)	0.011 (3)	0.011 (3)	0.014 (3)
Cd1	0.0309 (4)	0.0278 (4)	0.0387 (4)	0.0106 (2)	0.0152 (3)	0.0168 (3)
Br1	0.0350 (5)	0.0295 (5)	0.0480 (5)	0.0114 (4)	0.0154 (4)	0.0163 (4)
Br2	0.0306 (5)	0.0426 (6)	0.0383 (5)	0.0062 (4)	0.0109 (4)	0.0220 (4)
S1	0.0533 (15)	0.0470 (14)	0.0313 (11)	0.0098 (11)	0.0142 (10)	0.0205 (10)
S2	0.0375 (12)	0.0300 (11)	0.0378 (11)	0.0091 (9)	0.0129 (9)	0.0082 (9)

Geometric parameters (Å, º)

C1—C2	1.484 (14)	C6—H6	0.9300
C1—H1A	0.9600	C7—N2	1.298 (11)
C1—H1B	0.9600	C7—C8	1.505 (14)
C1—H1C	0.9600	C7—S2	1.717 (10)
C2—N1	1.329 (11)	C8—H8C	0.9600
C2—S1	1.719 (10)	C8—H8B	0.9600
C3—C4	1.343 (13)	C8—H8A	0.9600
C3—S1	1.703 (9)	Cd1—N1	2.435 (7)
C3—H3	0.9300	Cd1—N2	2.372 (7)
C4—N1	1.390 (11)	Cd1—Br1	2.7112 (11)
C4—C5	1.454 (11)	Cd1—Br2^{i}	2.7640 (12)
C5—C6	1.372 (12)	Cd1—Br1^{ii}	2.8362 (12)
C5—N2	1.397 (11)	Cd1—Br2	2.7845 (12)
C6—S2	1.693 (10)		
C2—C1—H1A	109.5	H8C—C8—H8A	109.5
C2—C1—H1B	109.5	H8B—C8—H8A	109.5
H1A—C1—H1B	109.5	C2—N1—C4	110.3 (8)
C2—C1—H1C	109.5	C2—N1—Cd1	135.3 (7)
H1A—C1—H1C	109.5	C4—N1—Cd1	114.0 (5)
H1B—C1—H1C	109.5	C7—N2—C5	110.7 (8)
N1—C2—C1	125.4 (9)	C7—N2—Cd1	134.0 (6)
N1—C2—S1	113.9 (7)	C5—N2—Cd1	115.2 (5)
C1—C2—S1	120.7 (7)	N2—Cd1—N1	71.9 (2)
C4—C3—S1	111.2 (7)	N2—Cd1—Br1	161.12 (17)
C4—C3—H3	124.4	N1—Cd1—Br1	96.12 (18)
S1—C3—H3	124.4	N2—Cd1—Br2^{i}	94.19 (17)
C3—C4—N1	114.9 (7)	N1—Cd1—Br2^{i}	84.58 (18)
C3—C4—C5	126.3 (8)	Br1—Cd1—Br2^{i}	99.26 (4)
N1—C4—C5	118.8 (7)	N2—Cd1—Br2	103.26 (18)
C6—C5—N2	114.2 (8)	N1—Cd1—Br2	168.62 (18)
C6—C5—C4	125.9 (8)	Br1—Cd1—Br2	91.01 (4)
N2—C5—C4	120.0 (7)	Br2^{i}—Cd1—Br2	85.52 (3)
C5—C6—S2	110.2 (7)	N2—Cd1—Br1^{ii}	82.02 (17)
C5—C6—H6	124.9	N1—Cd1—Br1^{ii}	98.39 (18)
S2—C6—H6	124.9	Br1—Cd1—Br1^{ii}	85.48 (4)
N2—C7—C8	124.8 (9)	Br2^{i}—Cd1—Br1^{ii}	174.15 (3)

N2—C7—S2	114.6 (7)	Br2—Cd1—Br1^{ii}	90.99 (3)
C8—C7—S2	120.6 (7)	Cd1—Br1—Cd1^{ii}	94.52 (4)
C7—C8—H8C	109.5	Cd1^{i}—Br2—Cd1	94.48 (3)
C7—C8—H8B	109.5	C3—S1—C2	89.8 (4)
H8C—C8—H8B	109.5	C6—S2—C7	90.3 (4)
C7—C8—H8A	109.5		

S1—C3—C4—N1	0.4 (10)	C7—N2—Cd1—Br2	14.8 (8)
S1—C3—C4—C5	−177.4 (7)	C5—N2—Cd1—Br2	−169.0 (5)
C3—C4—C5—C6	−6.7 (14)	C7—N2—Cd1—Br1^{ii}	−74.4 (8)
N1—C4—C5—C6	175.7 (8)	C5—N2—Cd1—Br1^{ii}	101.8 (5)
C3—C4—C5—N2	172.6 (8)	C2—N1—Cd1—N2	−174.0 (9)
N1—C4—C5—N2	−5.1 (11)	C4—N1—Cd1—N2	−2.8 (5)
N2—C5—C6—S2	0.1 (9)	C2—N1—Cd1—Br1	21.0 (9)
C4—C5—C6—S2	179.4 (7)	C4—N1—Cd1—Br1	−167.8 (5)
C1—C2—N1—C4	−179.4 (9)	C2—N1—Cd1—Br2^{i}	−77.8 (8)
S1—C2—N1—C4	−1.2 (10)	C4—N1—Cd1—Br2^{i}	93.4 (6)
C1—C2—N1—Cd1	−8.0 (15)	C2—N1—Cd1—Br2	−107.5 (11)
S1—C2—N1—Cd1	170.3 (5)	C4—N1—Cd1—Br2	63.8 (12)
C3—C4—N1—C2	0.5 (11)	C2—N1—Cd1—Br1^{ii}	107.3 (8)
C5—C4—N1—C2	178.5 (7)	C4—N1—Cd1—Br1^{ii}	−81.5 (6)
C3—C4—N1—Cd1	−172.9 (6)	N2—Cd1—Br1—Cd1^{ii}	48.6 (6)
C5—C4—N1—Cd1	5.0 (9)	N1—Cd1—Br1—Cd1^{ii}	97.98 (18)
C8—C7—N2—C5	−179.7 (10)	Br2^{i}—Cd1—Br1—Cd1^{ii}	−176.54 (3)
S2—C7—N2—C5	1.9 (10)	Br2—Cd1—Br1—Cd1^{ii}	−90.92 (4)
C8—C7—N2—Cd1	−3.4 (15)	Br1^{ii}—Cd1—Br1—Cd1^{ii}	0.0
S2—C7—N2—Cd1	178.2 (4)	N2—Cd1—Br2—Cd1^{i}	93.26 (18)
C6—C5—N2—C7	−1.3 (10)	N1—Cd1—Br2—Cd1^{i}	29.7 (9)
C4—C5—N2—C7	179.4 (7)	Br1—Cd1—Br2—Cd1^{i}	−99.21 (4)
C6—C5—N2—Cd1	−178.4 (6)	Br2^{i}—Cd1—Br2—Cd1^{i}	0.0
C4—C5—N2—Cd1	2.3 (9)	Br1^{ii}—Cd1—Br2—Cd1^{i}	175.30 (3)
C7—N2—Cd1—N1	−176.0 (9)	C4—C3—S1—C2	−0.8 (7)
C5—N2—Cd1—N1	0.2 (5)	N1—C2—S1—C3	1.2 (7)
C7—N2—Cd1—Br1	−123.4 (8)	C1—C2—S1—C3	179.5 (9)
C5—N2—Cd1—Br1	52.8 (9)	C5—C6—S2—C7	0.8 (7)
C7—N2—Cd1—Br2^{i}	101.1 (8)	N2—C7—S2—C6	−1.6 (8)
C5—N2—Cd1—Br2^{i}	−82.7 (5)	C8—C7—S2—C6	179.9 (9)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Br1^{iii}	0.93	2.87	3.754 (11)	159
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C8—H8*C*···Br2	0.96	2.74	3.681 (16)	167

Symmetry code: (iii) *x*, *y*+1, *z*.