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Bis[benzyl 3-(3-phenylprop-2-enyl-
idene)dithiocarbazato- κ^2N^3,S]cadmiumM. S. Reza,^a M. A. A. A. Islam,^a M. T. H. Tarafder,^{b*}
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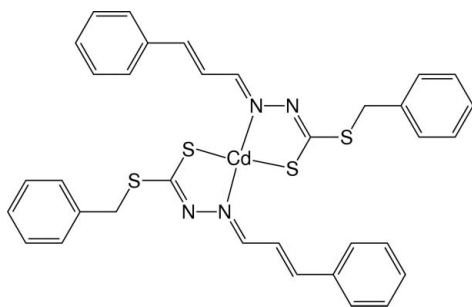
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.042; wR factor = 0.115; data-to-parameter ratio = 15.2.

In the title complex, $[Cd(C_{17}H_{15}N_2S_2)_2]$, the Cd^{II} ion is located on a twofold rotation axis and exhibits a coordination number of four within a very distorted coordination environment that is best described as bisphenoidal. The two deprotonated Schiff base ligands chelate the Cd^{II} ion through the azomethine N and the thiolate S atom. The dihedral angle between the two chelating ligands is $84.01(9)^\circ$. Weak intermolecular $C-H \cdots S$ interactions lead to the formation of chains along the c axis.

Related literature

For the structure of uncoordinated Schiff bases, see: Tarafder, Crouse *et al.* (2008); Tarafder, Islam *et al.* (2008). For the isotopic Zn and Hg analogues, see: Fun *et al.* (2008); Islam *et al.* (2012). For the coordination behaviour of metal ions (Co, Ni, Cu, Zn, Cd and Hg) with the cinnamaldehyde Schiff base of *S*-methylthiocarbazate, see: Liu *et al.* (2009); Abram *et al.* (2006). For the bioactivity of transition metal complexes of similar Schiff base ligands, see: Chew *et al.* (2004); How *et al.* (2008); Maia *et al.* (2010).



Experimental

Crystal data

$[Cd(C_{17}H_{15}N_2S_2)_2]$
 $M_r = 735.26$
Orthorhombic, $Pbcn$
 $a = 36.2497(7)$ Å
 $b = 9.9940(2)$ Å
 $c = 8.9392(2)$ Å

$V = 3238.49(12)$ Å³
 $Z = 4$
Cu $K\alpha$ radiation
 $\mu = 8.05$ mm⁻¹
 $T = 173$ K
 $0.3 \times 0.3 \times 0.1$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer
Absorption correction: multi-scan
(*ABSCOR*; Rigaku, 1995)
 $T_{min} = 0.325$, $T_{max} = 0.448$

10761 measured reflections
2964 independent reflections
2439 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.079$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.115$
 $S = 1.02$
2964 reflections

195 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 1.36$ e Å⁻³
 $\Delta\rho_{min} = -0.52$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cd—N1	2.306 (2)	Cd—S1	2.4285 (9)
N1 ⁱ —Cd—N1	103.00 (12)	N1—Cd—S1	80.27 (6)
N1 ⁱ —Cd—S1	119.99 (6)	S1—Cd—S1 ⁱ	149.19 (5)

Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C13—H13 ⁱⁱ \cdots S2 ⁱⁱ	0.95	2.75	3.690 (4)	170

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

Data collection: *RAPID-AUTO* (Rigaku, 1995); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2651).

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supplementary materials

Acta Cryst. (2012). E68, m976–m977 [doi:10.1107/S1600536812028127]

Bis[benzyl 3-(3-phenylprop-2-enylidene)dithiocarbazato- κ^2N^3,S]cadmium

M. S. Reza, M. A. A. A. Islam, M. T. H. Tarafder, M. C. Sheikh and E. Zangrando

Comment

In continuation of our interest in exploring the chemistry of Schiff bases derived from *S*-benzylthiocarbazate (Tarafder, Crouse *et al.*, 2008; Tarafder, Islam *et al.*, 2008) and of their metal complexes, due to their intriguing coordination behaviour, physico-chemical properties, and potential biological activities, we have completed the syntheses of group 12 metal complexes with the same Schiff base, *viz.* bis[benzyl *N'*-(3-phenylprop-2-enylidene)dithiocarbazate]. For the coordination behaviour of metal ions (Co, Ni, Cu, Zn, Cd, and Hg) with the cinnamaldehyde Schiff base of *S*-methylthiocarbazate, see: Liu *et al.* (2009); Abram *et al.*, (2006). For the bioactivity of transition metal complexes of similar Schiff base ligands, see: Chew *et al.* (2004); How *et al.* (2008); Maia *et al.* (2010).

In the present complex the Cd^{II} ion lies on a twofold rotation axis and therefore the asymmetric unit contains one-half of the molecule (Fig. 1). The fourfold coordination is best described as bisphenoidal, with the Cd^{II} ion being chelated by two benzyl *N'*-(3-phenylprop-2-enylidene)dithiocarbazate ligands through the azomethine nitrogen and the thiolate sulfur donors. The two chelating five-membered rings form a dihedral angle of 84.01 (9)°. Since the structure is isotopic with those of Zn (Fun *et al.*, 2008) and Hg (Islam *et al.*, 2012), it is worthwhile to compare the geometries around the metal ions. The *M*—N bond lengths in the series follow the trend Zn < Cd < Hg (2.0662 (12), 2.306 (2), 2.489 (3) Å) in agreement with the respective ionic radii. On the other hand, among the *M*—S bond lengths, the Cd—S one is the longest, with values of 2.2636 (4), 2.4285 (9), 2.3668 (11) Å along this series. Moreover, the bite angle N1—Cd—S1 of 80.27 (6)° is in between the values for the Zn (86.96 (3)°) and Hg (77.93 (6)°) complexes.

The crystal packing is consolidated by weak C13—H13···S2 interactions, giving rise to a chain motif extending along the *c* axis.

Experimental

The Schiff base, benzyl *N'*-(3-phenylprop-2-enylidene)hydrazinecarbodithioate was prepared as previously reported (Tarafder, Islam *et al.*, 2008). Cadmium(II) acetate dihydrate (0.066 g, 0.25 mmol) dissolved in absolute ethanol (20 ml) was added to a hot absolute ethanol solution (50 ml) of the Schiff base (0.163 g, 0.5 mmol) under refluxing condition, which was continued for 2 h. The yellow precipitate which formed was filtered off, washed with hot ethanol and dried *in vacuo* over anhydrous CaCl₂. Yield: 0.199 g (87%). 54 mg of the compound was dissolved in chloroform (10 ml) at room temperature and mixed with toluene (5 ml). The resultant solution was allowed to stand at ambient temperature. Yellow square-shaped flat single crystals developed after 7 days. (m.p.= 438 K).

Refinement

All H atoms were geometrically located and treated as riding atoms, with C—H = 0.95 Å for C(aromatic) and 0.99 Å, for C(methylene), with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest residual electron density peak (1.36 e Å⁻³) is located at 1.09 Å from the Cd atom.

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 1995); cell refinement: *RAPID-AUTO* (Rigaku, 1995); data reduction: *RAPID-AUTO* (Rigaku, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *publCIF* (Westrip, 2010).

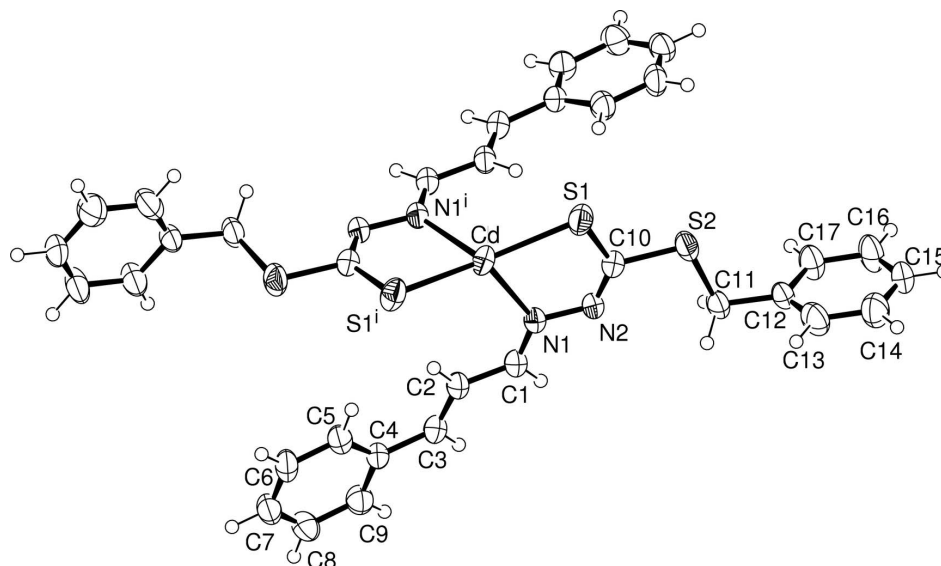


Figure 1

An ORTEP drawing (ellipsoids at the 50% probability level) of the title compound with the atom labelling scheme. [Symmetry code: (i) $-x + 1, y, -z + 3/2$.]

Bis[benzyl 3-(3-phenylprop-2-enylidene)dithiocarbazato- κ^2N^3,S]cadmium

Crystal data

$[\text{Cd}(\text{C}_{17}\text{H}_{15}\text{N}_2\text{S}_2)_2]$

$M_r = 735.26$

Orthorhombic, *Pbcn*

Hall symbol: $-P\ 2n\ 2ab$

$a = 36.2497(7)\ \text{\AA}$

$b = 9.9940(2)\ \text{\AA}$

$c = 8.9392(2)\ \text{\AA}$

$V = 3238.49(12)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1496$

$D_x = 1.508\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54187\ \text{\AA}$

Cell parameters from 29242 reflections

$\theta = 3.7\text{--}68.2^\circ$

$\mu = 8.05\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Prism, yellow

$0.3 \times 0.3 \times 0.1\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: $10.000\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*ABSCOR*; Rigaku, 1995)

$T_{\min} = 0.325, T_{\max} = 0.448$

10761 measured reflections

2964 independent reflections

2439 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.079$

$\theta_{\max} = 68.3^\circ, \theta_{\min} = 4.6^\circ$

$h = -42 \rightarrow 43$

$k = -11 \rightarrow 12$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
2964 reflections	$(\Delta/\sigma)_{\max} = 0.001$
195 parameters	$\Delta\rho_{\max} = 1.36 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.52 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd	0.5000	0.44301 (4)	0.7500	0.04150 (16)
N1	0.52779 (6)	0.2994 (3)	0.9175 (3)	0.0358 (6)
N2	0.56616 (6)	0.2968 (3)	0.9179 (3)	0.0367 (6)
S1	0.56402 (2)	0.50756 (11)	0.71527 (10)	0.0483 (3)
S2	0.62987 (2)	0.39583 (11)	0.83639 (11)	0.0540 (3)
C1	0.51250 (9)	0.2128 (3)	1.0048 (3)	0.0398 (7)
H1	0.5276	0.1511	1.0578	0.048*
C2	0.47320 (8)	0.2078 (3)	1.0235 (3)	0.0395 (7)
H2	0.4587	0.2715	0.9710	0.047*
C3	0.45573 (8)	0.1191 (4)	1.1103 (4)	0.0415 (8)
H3	0.4705	0.0526	1.1570	0.050*
C4	0.41607 (8)	0.1147 (3)	1.1403 (3)	0.0381 (7)
C5	0.39164 (8)	0.2100 (4)	1.0849 (4)	0.0436 (8)
H5	0.4007	0.2808	1.0244	0.052*
C6	0.35458 (8)	0.2033 (4)	1.1162 (4)	0.0476 (9)
H6	0.3383	0.2695	1.0779	0.057*
C7	0.34086 (9)	0.1000 (4)	1.2038 (4)	0.0511 (9)
H7	0.3152	0.0949	1.2243	0.061*
C8	0.36437 (11)	0.0055 (5)	1.2607 (4)	0.0516 (10)
H8	0.3550	-0.0643	1.3220	0.062*
C9	0.40186 (10)	0.0116 (5)	1.2288 (4)	0.0455 (8)
H9	0.4180	-0.0550	1.2675	0.055*
C10	0.58178 (8)	0.3856 (3)	0.8347 (3)	0.0391 (7)
C11	0.64403 (8)	0.2893 (4)	0.9912 (4)	0.0455 (8)
H11A	0.6300	0.3118	1.0829	0.055*
H11B	0.6399	0.1939	0.9668	0.055*

C12	0.68464 (8)	0.3169 (3)	1.0126 (3)	0.0413 (8)
C13	0.69639 (9)	0.4203 (4)	1.1010 (5)	0.0577 (10)
H13	0.6787	0.4747	1.1506	0.069*
C14	0.73377 (10)	0.4472 (4)	1.1193 (5)	0.0619 (12)
H14	0.7415	0.5188	1.1818	0.074*
C15	0.75932 (9)	0.3706 (4)	1.0474 (4)	0.0538 (10)
H15	0.7849	0.3884	1.0598	0.065*
C16	0.74806 (8)	0.2689 (4)	0.9579 (5)	0.0593 (10)
H16	0.7659	0.2167	0.9065	0.071*
C17	0.71095 (8)	0.2401 (4)	0.9404 (4)	0.0517 (9)
H17	0.7035	0.1675	0.8787	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.0334 (2)	0.0470 (3)	0.0440 (2)	0.000	-0.01208 (12)	0.000
N1	0.0262 (12)	0.0447 (16)	0.0365 (13)	0.0008 (11)	-0.0011 (10)	0.0027 (12)
N2	0.0255 (12)	0.0478 (17)	0.0368 (13)	0.0013 (11)	0.0000 (10)	0.0006 (12)
S1	0.0401 (5)	0.0524 (6)	0.0525 (5)	-0.0107 (4)	-0.0125 (4)	0.0125 (4)
S2	0.0278 (4)	0.0780 (7)	0.0562 (5)	-0.0073 (4)	0.0006 (3)	0.0214 (5)
C1	0.0286 (14)	0.050 (2)	0.0411 (16)	0.0016 (14)	-0.0024 (13)	0.0023 (15)
C2	0.0269 (14)	0.051 (2)	0.0408 (16)	0.0021 (14)	-0.0023 (12)	0.0052 (15)
C3	0.0308 (16)	0.052 (2)	0.0422 (17)	0.0037 (14)	-0.0054 (13)	0.0017 (15)
C4	0.0285 (15)	0.049 (2)	0.0368 (16)	-0.0030 (13)	-0.0014 (12)	-0.0023 (14)
C5	0.0337 (16)	0.049 (2)	0.0481 (18)	-0.0035 (14)	0.0000 (14)	0.0018 (16)
C6	0.0289 (16)	0.056 (2)	0.058 (2)	-0.0016 (15)	-0.0051 (14)	-0.0033 (18)
C7	0.0328 (18)	0.068 (3)	0.053 (2)	-0.0074 (17)	0.0038 (16)	-0.013 (2)
C8	0.044 (2)	0.058 (3)	0.054 (2)	-0.013 (2)	0.0063 (14)	0.0020 (17)
C9	0.0410 (19)	0.047 (2)	0.0486 (19)	0.0003 (17)	-0.0010 (14)	0.0020 (16)
C10	0.0301 (15)	0.049 (2)	0.0382 (16)	-0.0005 (14)	-0.0046 (12)	0.0002 (15)
C11	0.0256 (15)	0.060 (2)	0.0504 (19)	0.0024 (14)	0.0032 (13)	0.0102 (17)
C12	0.0256 (15)	0.055 (2)	0.0438 (17)	0.0007 (13)	0.0037 (12)	0.0050 (16)
C13	0.0376 (19)	0.071 (3)	0.065 (3)	0.0062 (17)	0.0113 (17)	-0.014 (2)
C14	0.046 (2)	0.075 (3)	0.065 (3)	-0.0093 (19)	-0.0016 (18)	-0.017 (2)
C15	0.0273 (16)	0.077 (3)	0.057 (2)	-0.0049 (17)	-0.0021 (15)	0.004 (2)
C16	0.0286 (18)	0.068 (3)	0.081 (3)	0.0077 (17)	0.0040 (16)	-0.010 (2)
C17	0.0330 (17)	0.054 (2)	0.068 (2)	0.0011 (15)	0.0028 (16)	-0.0126 (19)

Geometric parameters (\AA , $^\circ$)

Cd—N1 ⁱ	2.306 (2)	C6—H6	0.9500
Cd—N1	2.306 (2)	C7—C8	1.370 (6)
Cd—S1	2.4285 (9)	C7—H7	0.9500
Cd—S1 ⁱ	2.4285 (9)	C8—C9	1.390 (5)
N1—C1	1.291 (4)	C8—H8	0.9500
N1—N2	1.391 (3)	C9—H9	0.9500
N2—C10	1.288 (4)	C11—C12	1.510 (4)
S1—C10	1.744 (3)	C11—H11A	0.9900
S2—C10	1.746 (3)	C11—H11B	0.9900
S2—C11	1.819 (3)	C12—C13	1.368 (5)

C1—C2	1.435 (4)	C12—C17	1.384 (4)
C1—H1	0.9500	C13—C14	1.391 (4)
C2—C3	1.337 (4)	C13—H13	0.9500
C2—H2	0.9500	C14—C15	1.362 (5)
C3—C4	1.463 (4)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.356 (5)
C4—C5	1.392 (4)	C15—H15	0.9500
C4—C9	1.398 (5)	C16—C17	1.385 (4)
C5—C6	1.374 (4)	C16—H16	0.9500
C5—H5	0.9500	C17—H17	0.9500
C6—C7	1.388 (5)		
N1 ⁱ —Cd—N1	103.00 (12)	C7—C8—C9	120.2 (4)
N1 ⁱ —Cd—S1	119.99 (6)	C7—C8—H8	119.9
N1—Cd—S1	80.27 (6)	C9—C8—H8	119.9
N1 ⁱ —Cd—S1 ⁱ	80.27 (6)	C8—C9—C4	120.6 (4)
N1—Cd—S1 ⁱ	119.99 (6)	C8—C9—H9	119.7
S1—Cd—S1 ⁱ	149.19 (5)	C4—C9—H9	119.7
C1—N1—N2	114.6 (2)	N2—C10—S1	132.2 (2)
C1—N1—Cd	128.5 (2)	N2—C10—S2	118.3 (2)
N2—N1—Cd	116.73 (17)	S1—C10—S2	109.45 (17)
C10—N2—N1	115.2 (2)	C12—C11—S2	105.4 (2)
C10—S1—Cd	95.10 (11)	C12—C11—H11A	110.7
C10—S2—C11	104.71 (14)	S2—C11—H11A	110.7
N1—C1—C2	121.3 (3)	C12—C11—H11B	110.7
N1—C1—H1	119.3	S2—C11—H11B	110.7
C2—C1—H1	119.3	H11A—C11—H11B	108.8
C3—C2—C1	124.1 (3)	C13—C12—C17	118.2 (3)
C3—C2—H2	117.9	C13—C12—C11	121.0 (3)
C1—C2—H2	117.9	C17—C12—C11	120.8 (3)
C2—C3—C4	126.3 (3)	C12—C13—C14	121.1 (3)
C2—C3—H3	116.9	C12—C13—H13	119.4
C4—C3—H3	116.9	C14—C13—H13	119.4
C5—C4—C9	118.1 (3)	C15—C14—C13	119.9 (4)
C5—C4—C3	122.7 (3)	C15—C14—H14	120.1
C9—C4—C3	119.2 (3)	C13—C14—H14	120.1
C6—C5—C4	121.1 (3)	C16—C15—C14	119.6 (3)
C6—C5—H5	119.5	C16—C15—H15	120.2
C4—C5—H5	119.5	C14—C15—H15	120.2
C5—C6—C7	120.1 (3)	C15—C16—C17	121.0 (3)
C5—C6—H6	119.9	C15—C16—H16	119.5
C7—C6—H6	119.9	C17—C16—H16	119.5
C8—C7—C6	119.9 (3)	C12—C17—C16	120.1 (3)
C8—C7—H7	120.0	C12—C17—H17	119.9
C6—C7—H7	120.0	C16—C17—H17	119.9
N1 ⁱ —Cd—N1—C1	-62.5 (2)	C6—C7—C8—C9	-1.1 (6)
S1—Cd—N1—C1	178.8 (3)	C7—C8—C9—C4	0.8 (6)
S1 ⁱ —Cd—N1—C1	23.7 (3)	C5—C4—C9—C8	-0.3 (5)

N1 ⁱ —Cd—N1—N2	111.98 (19)	C3—C4—C9—C8	179.3 (3)
S1—Cd—N1—N2	-6.76 (17)	N1—N2—C10—S1	-2.2 (4)
S1 ⁱ —Cd—N1—N2	-161.87 (15)	N1—N2—C10—S2	176.47 (19)
C1—N1—N2—C10	-177.9 (3)	Cd—S1—C10—N2	-3.1 (3)
Cd—N1—N2—C10	6.8 (3)	Cd—S1—C10—S2	178.22 (14)
N1 ⁱ —Cd—S1—C10	-95.26 (13)	C11—S2—C10—N2	-10.3 (3)
N1—Cd—S1—C10	4.21 (13)	C11—S2—C10—S1	168.62 (18)
S1 ⁱ —Cd—S1—C10	138.83 (11)	C10—S2—C11—C12	-169.8 (2)
N2—N1—C1—C2	176.4 (2)	S2—C11—C12—C13	86.4 (3)
Cd—N1—C1—C2	-9.0 (4)	S2—C11—C12—C17	-92.0 (3)
N1—C1—C2—C3	178.8 (3)	C17—C12—C13—C14	-0.6 (6)
C1—C2—C3—C4	176.1 (3)	C11—C12—C13—C14	-179.1 (3)
C2—C3—C4—C5	-3.2 (5)	C12—C13—C14—C15	0.7 (6)
C2—C3—C4—C9	177.2 (3)	C13—C14—C15—C16	0.2 (6)
C9—C4—C5—C6	0.1 (5)	C14—C15—C16—C17	-1.1 (6)
C3—C4—C5—C6	-179.5 (3)	C13—C12—C17—C16	-0.2 (5)
C4—C5—C6—C7	-0.3 (5)	C11—C12—C17—C16	178.2 (3)
C5—C6—C7—C8	0.8 (5)	C15—C16—C17—C12	1.1 (6)

Symmetry code: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C13—H13 \cdots S2 ⁱⁱ	0.95	2.75	3.690 (4)	170

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