# metal-organic compounds

# Bis[benzyl 3-(3-phenylprop-2-enyl-idene)dithiocarbazato-$\kappa^2 N^3$,$S$]cadmium

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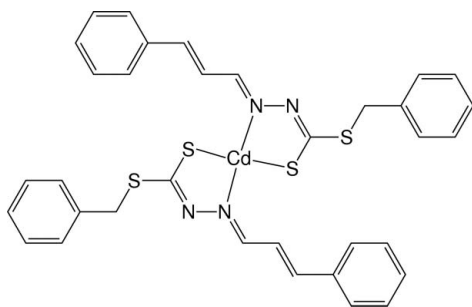Correspondence e-mail: ttofazzal@yahoo.com

In the title complex, [Cd(C$_{17}$H$_{15}$N$_2$S$_2$)$_2$], 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)°. Weak intermolecular C—H···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 isotypic 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*-methyldithiocarbazate, 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$_2$S$_2$)$_2$] | $V$ = 3238.49 (12) Å$^3$ |
| $M_r$ = 735.26 | $Z$ = 4 |
| Orthorhombic, $Pbcn$ | Cu $K\alpha$ radiation |
| $a$ = 36.2497 (7) Å | $\mu$ = 8.05 mm$^{-1}$ |
| $b$ = 9.9940 (2) Å | $T$ = 173 K |
| $c$ = 8.9392 (2) Å | 0.3 × 0.3 × 0.1 mm |

### Data collection

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 10761 measured reflections |
| Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995) | 2964 independent reflections |
| $T_{min}$ = 0.325, $T_{max}$ = 0.448 | 2439 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.079 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | 195 parameters |
| $wR(F^2)$ = 0.115 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 1.36 e Å$^{-3}$ |
| 2964 reflections | $\Delta\rho_{min}$ = −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···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C13—H13···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).

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

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## supporting information

## Bis[benzyl 3-(3-phenylprop-2-enylidene)dithiocarbazato-*κ²N³,S*]cadmium

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

### S1. Comment

In continuation of our interest in exploring the chemistry of Schiff bases derived from *S*-benzyldithiocarbazate (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*-methyl-dithiocarbazate, 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 isotypic 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.

### S2. Experimental

The Schiff base, benzyl *N′*-(3-phenylprop-2-enylidene)hydrazinecarbodithioate was prepared as prevoiusly 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 CaCl$_2$. 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).

### S3. 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) = 1.2$U_{eq}$(C). The highest residual electron density peak (1.36 e Å$^{-3}$) is located at 1.09 Å from the Cd atom.
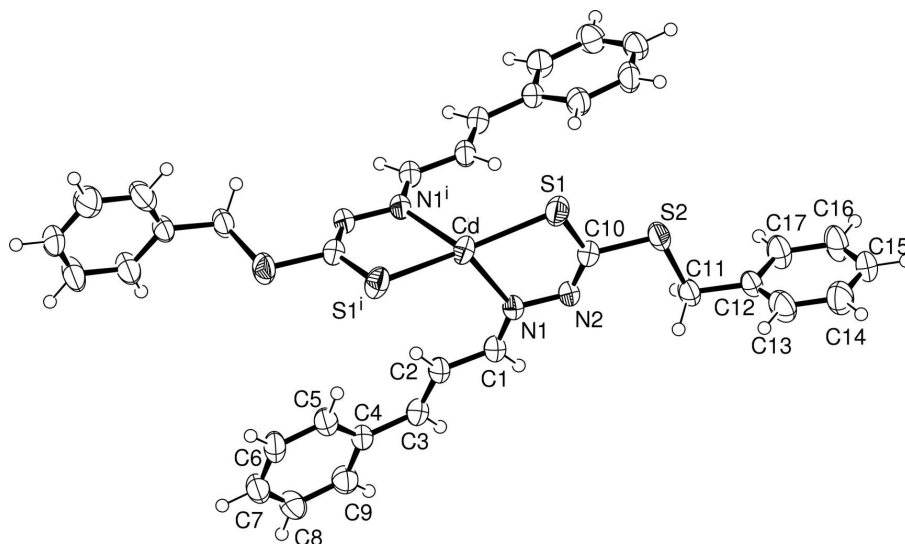
**Figure 1**

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- $\kappa^2 N^3$,*S*]cadmium**

*Crystal data*

| | |
|---|---|
| [Cd(C$_{17}$H$_{15}$N$_2$S$_2$)$_2$] | $F(000) = 1496$ |
| $M_r = 735.26$ | $D_x = 1.508$ Mg m$^{-3}$ |
| Orthorhombic, *Pbcn* | Cu *Kα* radiation, $\lambda = 1.54187$ Å |
| Hall symbol: -P 2n 2ab | Cell parameters from 29242 reflections |
| $a = 36.2497$ (7) Å | $\theta = 3.7–68.2°$ |
| $b = 9.9940$ (2) Å | $\mu = 8.05$ mm$^{-1}$ |
| $c = 8.9392$ (2) Å | $T = 173$ K |
| $V = 3238.49$ (12) Å$^3$ | Prism, yellow |
| $Z = 4$ | 0.3 × 0.3 × 0.1 mm |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID diffractometer | 10761 measured reflections |
| Radiation source: fine-focus sealed tube | 2964 independent reflections |
| Graphite monochromator | 2439 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.000 pixels mm$^{-1}$ | $R_{int} = 0.079$ |
| *ω* scans | $\theta_{max} = 68.3°$, $\theta_{min} = 4.6°$ |
| Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995) | $h = -42 \rightarrow 43$ |
| | $k = -11 \rightarrow 12$ |
| $T_{min} = 0.325$, $T_{max} = 0.448$ | $l = -10 \rightarrow 10$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | 0 restraints |
| Least-squares matrix: full | Primary atom site location: structure-invariant direct methods |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | |
| $wR(F^2) = 0.115$ | Secondary atom site location: difference Fourier map |
| $S = 1.02$ | |
| 2964 reflections | Hydrogen site location: inferred from neighbouring sites |
| 195 parameters | |

| H-atom parameters constrained | $(\Delta/\sigma)_{max} = 0.001$ |
| $w = 1/[\sigma^2(F_o^2) + (0.0606P)^2]$ | $\Delta\rho_{max} = 1.36$ e Å$^{-3}$ |
| where $P = (F_o^2 + 2F_c^2)/3$ | $\Delta\rho_{min} = -0.52$ e Å$^{-3}$ |

*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 (Å²)*

|  | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| 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) | | |
| | | | |
| N1i—Cd—N1 | 103.00 (12) | C7—C8—C9 | 120.2 (4) |
| N1i—Cd—S1 | 119.99 (6) | C7—C8—H8 | 119.9 |
| N1—Cd—S1 | 80.27 (6) | C9—C8—H8 | 119.9 |
| N1i—Cd—S1i | 80.27 (6) | C8—C9—C4 | 120.6 (4) |
| N1—Cd—S1i | 119.99 (6) | C8—C9—H9 | 119.7 |
| S1—Cd—S1i | 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 |
| | | | |
| N1i—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) |
| S1i—Cd—N1—C1 | 23.7 (3) | C5—C4—C9—C8 | −0.3 (5) |
| N1i—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) |
| S1i—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) |
| N1ⁱ—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) |
| S1ⁱ—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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C13—H13···S2ⁱⁱ | 0.95 | 2.75 | 3.690 (4) | 170 |

Symmetry code: (ii) *x*, −*y*+1, *z*+1/2.