

Received 19 July 2017

Accepted 7 August 2017

Edited by M. Zeller, Purdue University, USA

Keywords: crystal structure; cadmium(II) complex; *N,N*-diallyldithiocarbamate ligands; bridging dimeric structure.

CCDC reference: 899314

Supporting information: this article has supporting information at journals.iucr.org/e

Bis(μ -*N,N*-diallyldithiocarbamato)bis[(*N,N*-diallyldithiocarbamato)cadmium]

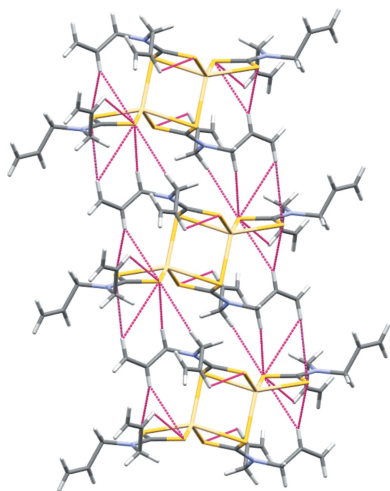
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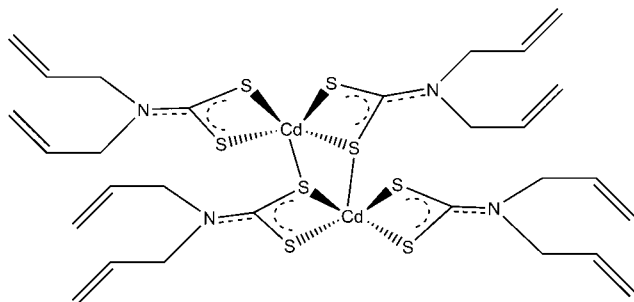
The title compound, [Cd₂(C₇H₁₀NS₂)₄], is a neutral dinuclear cadmium(II) complex bearing four bis *N,N*-diallyldithiocarbamate ligands coordinating to two Cd^{II} cations. In each of the monomeric subunits, there are four S atoms of two dithiocarbamate ligands [Cd–S = 2.5558 (3), 2.8016 (3), 2.6050 (3) and 2.5709 (3) Å] that coordinate to one Cd^{II} atom in a bidentate mode. The dimers are located over an inversion centre bridged by two additional bridging Cd–S bonds [2.6021 (3) Å], leading to a substantial distortion of the geometry of the monomeric subunit from the expected square-planar geometry. The five-coordinate environment around each of the Cd^{II} ions in the dimer is best described as substantially tetragonally distorted square pyramidal. The dithiocarbamate groups are themselves planar and are also coplanar with the Cd^{II} ions. The negative charge on these groups is delocalized by resonance across the S atoms bound to the Cd^{II} cation. This delocalization of the π electrons in the dithiocarbamate groups also extends to the C–N bonds as they reveal significant double bond character [C–N = 1.3213 (16) and 1.3333 (15) Å].

1. Chemical context

Interest in the study of metal dithiocarbamates was aroused because of their interesting structural features and diverse applications (Thammakan & Somsook, 2006). Dithiocarbamate complexes have largely been prepared from the group 12 elements, mostly because they have found wide practical application as additives to pavement asphalt, as antioxidants, and as potent pesticides *etc* (Subha *et al.*, 2010). The structural chemistry of cadmium dithiocarbamates of the general formula Cd(S₂CNRR') where R, R' = alkyl or aryl is dominated by its existence in binuclear form. This common feature has been ascribed to the effect of aggregated species, which they adopt in the solid state, resulting from equal numbers of μ_2 -tridentate and bidentate (chelating) ligands (Tiekink, 2003; Tan, Halim *et al.*, 2016). Only a few exceptions have been reported where the complex exists in a trinuclear form (Kumar *et al.*, 2014), or as a one-dimensional polymeric motif (Tan *et al.*, 2013, 2016; Ferreira *et al.*, 2016). Bis(*N,N*-diallyldithiocarbamato)cadmium compounds have the advantage of having stability similar to that of the zinc complexes, but more favourable stability when compared to the mercury complexes. Cadmium dithiocarbamate complexes have been widely used as single-source precursors for CdS



nanoparticles and thin films, which have application as non-linear optical materials (Thammakan & Somsook, 2006). Another important practical application of cadmium dithiocarbamates is their ability to efficiently collect gold from acidic solutions (Rodina *et al.*, 2014). Here we describe the crystal structure of a Cd^{II} complex bearing a diallyldithiocarbamate ligand in a chelating and bridging dimeric structure.



2. Structural commentary

The coordination environment of the Cd^{II} cation is observed to have a distorted tetragonal-pyramidal geometry (Fig. 1). The Cd^{II} cation is coordinated by four S atoms with distances ranging from 2.5558 (3) to 2.8016 (3) Å and to a fifth S atom at a distance of 2.6021 (3) Å; these distances are similar to other complexes found to have been published previously (see Section 4: *Database survey*). A full geometry check carried out with the *Mogul* Geometry Check tool (Bruno *et al.*, 2004) within the CSD suite of programs, showed no unusual geometrical parameters. The fifth S atom, S12^{i} , is from a third ligand that is in the coordination sphere of a centrosymmetrically related Cd^{II} ion [symmetry code: (i) $-x + 2, -y, -z + 1$]. This means that each bridging S atom simultaneously occupies an equatorial coordination site on one Cd^{II} ion and an apical site on the other Cd^{II} ion to form an edge-shared tetragonal-pyramidal geometry. The Cd^{II} ion deviates from the $\text{S11}-\text{S12}-\text{S22}-\text{S21}$ mean plane by 0.704016 (17) Å towards S12^{i} . The bridging network $\text{Cd1}-\text{S12}-\text{Cd1}^{\text{i}}-\text{S12}^{\text{i}}$ is completely

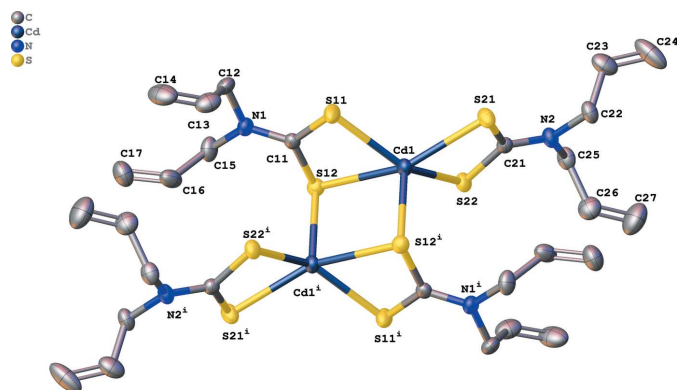


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering scheme [symmetry code: (i) $-x + 2, -y, -z + 1$]. H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Cd1—S11	2.5558 (3)	S12—C11	1.7532 (13)
Cd1—S22	2.5709 (3)	S21—C21	1.7224 (12)
Cd1—S12 ⁱ	2.6021 (3)	S22—C21	1.7263 (12)
Cd1—S21	2.6050 (3)	N1—C11	1.3213 (16)
Cd1—S12	2.8016 (3)	N2—C21	1.3333 (15)
S11—C11	1.7162 (13)		
S11—Cd1—S22	143.705 (13)	S22—Cd1—S12	96.950 (10)
S11—Cd1—S21	108.203 (11)	S12 ⁱ —Cd1—S12	96.257 (9)
S22—Cd1—S21	70.264 (10)	S21—Cd1—S12	152.651 (11)
S11—Cd1—S12	67.486 (10)	Cd1 ⁱ —S12—Cd1	83.743 (9)

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

planar since it lies over the inversion centre with a $\text{Cd1} \cdots \text{Cd1}^{\text{i}}$ separation distance of 3.60987 (8) Å and $\text{S12}-\text{Cd1}-\text{S12}^{\text{i}}$ and $\text{Cd1}-\text{S12}-\text{Cd1}^{\text{i}}$ angles of 96.257 (9) and 83.743 (9)°, respectively. There is substantial distortion of the geometry of the monomeric subunit from the expected square-planar geometry. Deviations from the standard 90° angles are evident in the angles of $\text{S11}-\text{Cd1}-\text{S21}$ [108.203 (11)°]; $\text{S22}-\text{Cd1}-\text{S21}$ [70.264 (10)°]; $\text{S22}-\text{Cd1}-\text{S12}$ [96.950 (10)°] and $\text{S11}-\text{Cd1}-\text{S12}$ [67.486 (10)°]. Deviations in the standard 180° angles are evident in the angles of $\text{S11}-\text{Cd1}-\text{S22}$ [143.705 (13)°] and $\text{S21}-\text{Cd1}-\text{S12}$ [152.651 (11)°]. The $\text{Cd1}-\text{S12}-\text{Cd1}^{\text{i}}-\text{S12}^{\text{i}}$ and $\text{S11}-\text{S12}-\text{S22}-\text{S21}$ mean planes form a dihedral (twist) angle of 84.6228 (18)°. The dithiocarbamate groups are planar and each group of the monomeric subunit is coplanar with the Cd^{II} ion (r.m.s. deviation is 0.010 Å). The mean plane consisting of atoms Cd1, S11, N1, C11, S12 and the mean plane consisting of atoms Cd1, S22, N2, C21, S21 have a plane-normal-to-plane-normal angle of 37.0291 (10)°; a centroid-to-centroid distance of 4.45354 (8) Å; a plane-to-plane shift of 4.22298 (8) Å and a plane-to-plane torsion (twist) angle of 8.0304 (12)°.

The $\text{S12}-\text{C11}$ bond length [1.7532 (13) Å] is longer than the adjacent $\text{S11}-\text{C11}$ bond length [1.7162 (13) Å] suggesting that this bond has more double bond character in the dithiocarbamate portion that coordinates to the Cd^{II} cation. On the opposite side of the Cd^{II} ion, both S—C bonds have approximately the same length, where $\text{S21}-\text{C21}$ and $\text{S22}-\text{C21}$ bond lengths are 1.7224 (12) and 1.7263 (12) Å, respectively, suggesting that the double bond of the dithiocarbamate is spread over the S—C—S bond *via* resonance. A possible explanation for this may be because of the fact that atom S12 serves as the bridging S atom in the complex. Also, the $\text{N1}-\text{C11}$ and $\text{N2}-\text{C21}$ distances [1.3213 (16) and 1.3333 (15) Å, respectively] are shorter compared to the other N—C distances indicating considerable double-bond character. The vinyl substituents are also planar and are at an angle of 91.6049 (14)° from the dithiocarbamate plane and at an angle of 150.9196 (6)° from the vinyl group directly opposite from it. This scenario is comparable with the other structures surveyed in the literature (see Section 4: *Database survey*). All highlighted and discussed geometrical parameters describing the coordination environment are given in Table 1. Weak intramolecular C—H $\cdots$ S interactions are observed (Table 2)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12B $\cdots$ S11	0.99	2.59	2.9783 (14)	103
C15—H15A $\cdots$ S12	0.99	2.50	3.0438 (14)	115
C22—H22B $\cdots$ S21	0.99	2.50	3.0381 (13)	114
C25—H25B $\cdots$ S22	0.99	2.56	2.9845 (14)	106

3. Supramolecular features

The space group of the crystal is $P\bar{1}$, and the asymmetric unit consists of one-half of the complex molecule, so that the unit cell contains one complete complex molecule. Each half of the asymmetric unit is related by an inversion centre. In the crystal, weak C—H $\cdots\pi$ interactions are observed, forming chains along [001] (see Fig. 2 and Table 3).

4. Database survey

A search of the Cambridge Structural Database (version 1.19, May 2017 updates) (Groom *et al.*, 2016) revealed that there are a number of similar types of compounds where in place of the *N,N*-diallyl side chain, the side-chains substituents are di-*n*-propyl [CSD refcodes BEHNOR (Jian *et al.*, 1999a),

Table 3
 $X-H\cdots\pi$ interactions.

Cg3 is the centroid of the Cd1—S11—C11—S12—Cd1ⁱ—S12ⁱ ring.

$C-H\cdots Cg$	$C-H$	$H\cdots Cg$	$C\cdots Cg$	$C-H\cdots Cg$
C15—H15B $\cdots$ Cg3	0.99	2.94	3.9209 (17)	171
C16—H16 $\cdots$ Cg3	0.99	2.90	3.7648 (17)	152

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

BEHNOR01 (Ivanov *et al.*, 2005)], di-isobutyl [LESVEK (Cox & Tiekink, 1999), LESVEK01 (Glinskaya *et al.*, 1999)] and di-isopropyl [SUVTUY (Jian *et al.*, 1999b), SUVTUY01 (Cox & Tiekink, 1999)].

5. Synthesis and crystallization

A solution of $CdCl_2 \cdot 2H_2O$ (0.55 g, 0.0025 mol) in ethanol (10 ml) was added to a solution of sodium *N,N*-diallyl di-thiocarbamate (0.98 g, 0.005 mol) in ethanol (10 ml), and the resulting suspension was stirred for 45 min at room temperature. This solution was then filtered, and rinsed several times with distilled water (Onwudiwe *et al.*, 2015) and ethanol. Yield: 1.28 g, 56%. Analysis found: C, 36.38; H, 4.40; N, 6.50; S, 28.42%. Calculated for $C_{14}H_{20}N_2S_4Cd$: C, 36.79; H, 4.41; N, 6.13; S, 28.06. Crystals suitable for single-crystal X-ray analysis were obtained by recrystallization from chloroform/ethanol. Other analytical data for this material (melting point, IR and

Table 4
Experimental details.

Crystal data	
Chemical formula	$[Cd_2(C_7H_{10}NS_2)_4]$
M_r	913.92
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	200
a, b, c (Å)	8.0872 (2), 9.4146 (2), 13.0721 (3)
α, β, γ (°)	75.858 (1), 78.460 (1), 77.488 (1)
V (Å ³)	930.75 (4)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.62
Crystal size (mm)	0.60 $\times$ 0.44 $\times$ 0.17
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Numerical (SADABS; Bruker, 2011)
T_{min}, T_{max}	0.824, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16101, 4644, 4391
R_{int}	0.015
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.015, 0.037, 1.15
No. of reflections	4644
No. of parameters	191
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.28, -0.31

Computer programs: *BIS* and *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2017* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

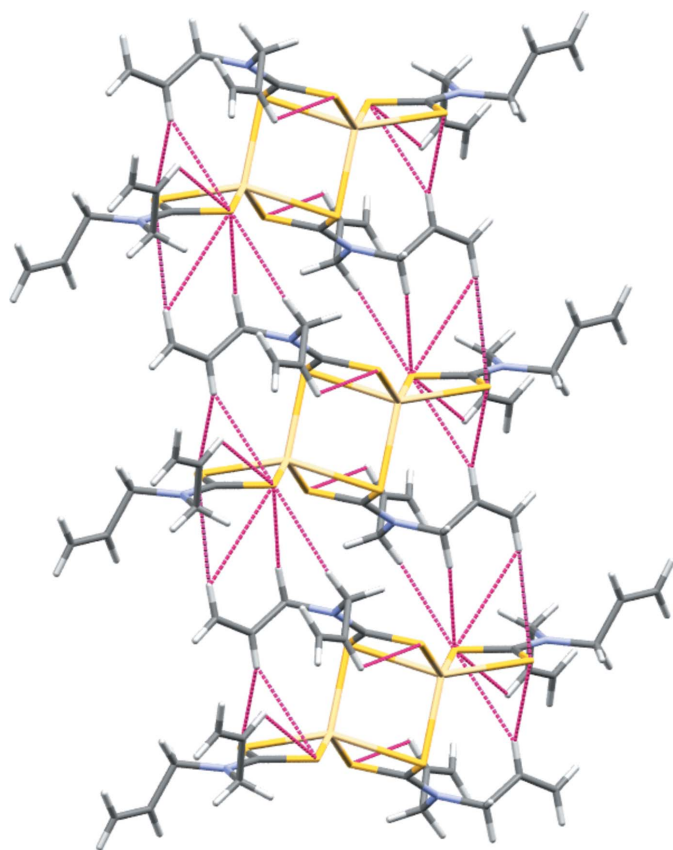


Figure 2
The crystal structure of the title compound constructed from chains formed by C—H $\cdots$ S interactions (red dashed lines). [Authors: Please add unit cell outline and coordinate axes]

NMR data) has been published previously (Onwudiwe *et al.*, 2015).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms were positioned geometrically and refined isotropically using the riding-model approximation with C—H = 0.99 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for methylene groups and C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for all vinyl groups.

Acknowledgements

The authors wish to acknowledge their respective institutions for their facilities to carry out the synthesis and characterization of the title compound.

Funding information

Funding for this research was provided by: North-West University, South Africa.

References

- Bruker (2009). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2011). *BIS*, *APEX2* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruno, I. J., Cole, J. C., Kessler, M., Luo, J., Motherwell, S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.
- Cox, M. J. & Tiekink, E. R. T. (1999). *Z. Kristallogr.* **214**, 670–676.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Ferreira, I. P., de Lima, G. M., Paniago, E. B., Pinheiro, C. B., Wardell, J. L. & Wardell, S. M. S. V. (2016). *Inorg. Chim. Acta*, **441**, 137–145.
- Glinskaya, L. A., Zemskova, S. M. & Klevtsova, R. F. (1999). *Zh. Strukt. Khim. (Russ. J. Struct. Chem.)*, **40**, 979–983.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Ivanov, A. V., Konzelko, A. A., Gerasimenko, A. V., Ivanov, M. A., Antsutkin, O. N. & Forsling, W. (2005). *Russ. J. Inorg. Chem.* **50**, 1827.
- Jian, F., Wang, Z., Bai, Z., You, X., Fun, H. & Chinnakali, K. (1999a). *J. Chem. Crystallogr.* **29**, 227–231.
- Jian, F.-F., Wang, Z.-X., Fun, H.-K., Bai, Z.-P. & You, X.-Z. (1999b). *Acta Cryst.* **C55**, 174–176.
- Kumar, V., Singh, V., Gupta, A. N., Manar, K. K., Drew, M. G. B. & Singh, N. (2014). *CrystEngComm*, **16**, 6765–6774.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Onwudiwe, D. C., Hrubaru, M. & Ebenso, E. E. (2015). *J. Nanomaterials*, **2015**, 1–9.
- Rodina, T. A., Ivanov, A. V. & Gerasimenko, A. V. (2014). *Russ. J. Coord. Chem.* **40**, 100–108.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Subha, P. V., Valarmathi, P., Srinivasan, N., Thirumaran, S. & Saminathan, K. (2010). *Polyhedron*, **29**, 1078–1082.
- Tan, Y. S., Halim, S. N. A. & Tiekink, E. R. T. (2016). *Z. Kristallogr.* **231**, 113–126.
- Tan, Y. S., Sudlow, A. L., Molloy, K. C., Morishima, Y., Fujisawa, K., Jackson, W. J., Henderson, W., Halim, S. N. B. A., Ng, S. W. & Tiekink, E. R. T. (2013). *Cryst. Growth Des.* **13**, 3046–3056.
- Thammakan, N. & Somsook, E. (2006). *Mater. Lett.* **60**, 1161–1165.
- Tiekink, E. R. T. (2003). *CrystEngComm*, **5**, 101–113.

supporting information

Acta Cryst. (2017). E73, 1353-1356 [https://doi.org/10.1107/S2056989017011616]

Bis(μ -*N,N*-diallyldithiocarbamato)bis[(*N,N*-diallyldithiocarbamato)cadmium]

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Computing details

Data collection: *BIS* (Bruker, 2011); cell refinement: *APEX2* (Bruker, 2011); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

Bis(μ -*N,N*-diallyldithiocarbamato)bis[(*N,N*-diallyldithiocarbamato)cadmium]

Crystal data

[Cd₂(C₇H₁₀NS₂)₄]
 $M_r = 913.92$
 Triclinic, $P\bar{1}$
 $a = 8.0872$ (2) Å
 $b = 9.4146$ (2) Å
 $c = 13.0721$ (3) Å
 $\alpha = 75.858$ (1)°
 $\beta = 78.460$ (1)°
 $\gamma = 77.488$ (1)°
 $V = 930.75$ (4) Å³

$Z = 1$
 $F(000) = 460$
 $D_x = 1.631$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 9892 reflections
 $\theta = 3.1$ – 28.4°
 $\mu = 1.62$ mm⁻¹
 $T = 200$ K
 Platelet, colourless
 $0.60 \times 0.44 \times 0.17$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: sealed tube
 Graphite monochromator
 Detector resolution: 8.3333 pixels mm⁻¹
 φ and ω scans
 Absorption correction: numerical
 (SADABS; Bruker, 2011)
 $T_{\min} = 0.824$, $T_{\max} = 1.000$

16101 measured reflections
 4644 independent reflections
 4391 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 2.5^\circ$
 $h = -10 \rightarrow 10$
 $k = -12 \rightarrow 12$
 $l = -16 \rightarrow 17$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.015$
 $wR(F^2) = 0.037$
 $S = 1.15$
 4644 reflections
 191 parameters
 0 restraints
 Primary atom site location: dual

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0111P)^2 + 0.3546P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.28$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

Extinction correction: SHELXL2017
 (Sheldrick, 2015),
 $F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0173 (7)

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. Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 $U_{eq}(C)$.
 Two reflections with large differences between their observed and calculated intensity were omitted. This is probably due to obstruction by the beam stop.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Cd1	0.89235 (2)	−0.00613 (2)	0.63560 (2)	0.02744 (4)
S11	0.78076 (5)	−0.22154 (4)	0.60114 (3)	0.03471 (8)
S12	0.78142 (4)	0.06086 (3)	0.43671 (3)	0.02551 (7)
S21	0.84065 (5)	−0.02186 (4)	0.84095 (3)	0.03026 (7)
S22	0.80123 (4)	0.25713 (4)	0.67413 (2)	0.02688 (7)
N1	0.66681 (14)	−0.17652 (12)	0.41751 (9)	0.0263 (2)
N2	0.76538 (14)	0.25083 (12)	0.88135 (8)	0.0252 (2)
C11	0.73731 (15)	−0.12060 (14)	0.47817 (10)	0.0234 (2)
C12	0.61897 (18)	−0.32572 (16)	0.45381 (11)	0.0323 (3)
H12A	0.522086	−0.328088	0.418787	0.039*
H12B	0.579076	−0.343192	0.531802	0.039*
C13	0.7621 (2)	−0.44839 (16)	0.43028 (13)	0.0402 (3)
H13	0.865773	−0.457570	0.456951	0.048*
C14	0.7529 (3)	−0.54414 (18)	0.37491 (16)	0.0535 (5)
H14A	0.650843	−0.537598	0.347257	0.064*
H14B	0.848334	−0.620204	0.362346	0.064*
C15	0.6278 (2)	−0.09675 (16)	0.31078 (11)	0.0342 (3)
H15A	0.641253	0.008254	0.299629	0.041*
H15B	0.506864	−0.097581	0.307348	0.041*
C16	0.74035 (18)	−0.16349 (18)	0.22396 (11)	0.0367 (3)
H16	0.860609	−0.180714	0.223617	0.044*
C17	0.6869 (2)	−0.2001 (2)	0.14846 (13)	0.0468 (4)
H17A	0.567516	−0.184585	0.146136	0.056*
H17B	0.767061	−0.242477	0.095478	0.056*
C21	0.79907 (15)	0.16963 (13)	0.80674 (10)	0.0221 (2)
C22	0.78373 (18)	0.18663 (15)	0.99407 (10)	0.0302 (3)
H22A	0.861484	0.238077	1.015705	0.036*
H22B	0.836930	0.080256	1.001404	0.036*
C23	0.6172 (2)	0.19957 (18)	1.06666 (12)	0.0420 (4)
H23	0.528018	0.158623	1.053323	0.050*
C24	0.5865 (3)	0.2647 (2)	1.14844 (14)	0.0635 (6)

H24A	0.673453	0.306597	1.163574	0.076*
H24B	0.477492	0.269906	1.192382	0.076*
C25	0.72097 (18)	0.41463 (14)	0.85522 (11)	0.0307 (3)
H25A	0.640375	0.449151	0.915541	0.037*
H25B	0.662323	0.445861	0.791634	0.037*
C26	0.8754 (2)	0.48598 (16)	0.83349 (13)	0.0407 (3)
H26	0.964495	0.461004	0.777955	0.049*
C27	0.8956 (3)	0.5809 (2)	0.88618 (19)	0.0629 (5)
H27A	0.808789	0.608066	0.942160	0.075*
H27B	0.997242	0.622596	0.868496	0.075*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02830 (6)	0.03364 (6)	0.02419 (6)	−0.00931 (4)	−0.00001 (4)	−0.01311 (4)
S11	0.0509 (2)	0.03708 (18)	0.02178 (15)	−0.02237 (16)	−0.00800 (14)	−0.00194 (13)
S12	0.02576 (15)	0.02429 (14)	0.02685 (15)	−0.00332 (11)	−0.00321 (12)	−0.00771 (11)
S21	0.04427 (19)	0.02305 (14)	0.02257 (15)	−0.00670 (13)	−0.00156 (13)	−0.00538 (11)
S22	0.03366 (16)	0.02749 (15)	0.02034 (14)	−0.00547 (12)	−0.00683 (12)	−0.00441 (11)
N1	0.0255 (5)	0.0302 (5)	0.0262 (5)	−0.0061 (4)	−0.0051 (4)	−0.0093 (4)
N2	0.0296 (5)	0.0239 (5)	0.0214 (5)	0.0007 (4)	−0.0052 (4)	−0.0070 (4)
C11	0.0198 (5)	0.0288 (6)	0.0225 (5)	−0.0051 (4)	0.0005 (4)	−0.0093 (5)
C12	0.0311 (7)	0.0389 (7)	0.0328 (7)	−0.0180 (6)	−0.0036 (5)	−0.0096 (6)
C13	0.0388 (8)	0.0292 (7)	0.0493 (9)	−0.0108 (6)	−0.0098 (7)	0.0045 (6)
C14	0.0623 (11)	0.0312 (8)	0.0604 (11)	−0.0166 (7)	0.0138 (9)	−0.0086 (7)
C15	0.0404 (8)	0.0328 (7)	0.0330 (7)	0.0007 (6)	−0.0179 (6)	−0.0098 (6)
C16	0.0267 (6)	0.0527 (9)	0.0279 (7)	−0.0097 (6)	−0.0037 (5)	−0.0010 (6)
C17	0.0537 (10)	0.0539 (10)	0.0336 (8)	−0.0058 (8)	−0.0040 (7)	−0.0163 (7)
C21	0.0188 (5)	0.0252 (6)	0.0227 (5)	−0.0039 (4)	−0.0028 (4)	−0.0064 (4)
C22	0.0365 (7)	0.0318 (6)	0.0212 (6)	0.0017 (5)	−0.0062 (5)	−0.0089 (5)
C23	0.0427 (8)	0.0414 (8)	0.0309 (7)	−0.0007 (7)	0.0002 (6)	0.0023 (6)
C24	0.0823 (14)	0.0469 (10)	0.0345 (9)	0.0170 (10)	0.0156 (9)	−0.0033 (7)
C25	0.0376 (7)	0.0243 (6)	0.0286 (6)	0.0035 (5)	−0.0072 (5)	−0.0091 (5)
C26	0.0487 (9)	0.0285 (7)	0.0445 (9)	−0.0070 (6)	−0.0074 (7)	−0.0067 (6)
C27	0.0769 (14)	0.0452 (10)	0.0796 (14)	−0.0149 (9)	−0.0308 (12)	−0.0187 (10)

Geometric parameters ($\text{\AA}$, $^\circ$)

Cd1—S11	2.5558 (3)	C15—C16	1.483 (2)
Cd1—S22	2.5709 (3)	C15—H15A	0.9900
Cd1—S12 ⁱ	2.6021 (3)	C15—H15B	0.9900
Cd1—S21	2.6050 (3)	C16—C17	1.297 (2)
Cd1—S12	2.8016 (3)	C16—H16	0.9500
S11—C11	1.7162 (13)	C17—H17A	0.9500
S12—C11	1.7532 (13)	C17—H17B	0.9500
S21—C21	1.7224 (12)	C22—C23	1.484 (2)
S22—C21	1.7263 (12)	C22—H22A	0.9900
N1—C11	1.3213 (16)	C22—H22B	0.9900

N1—C15	1.4735 (17)	C23—C24	1.315 (3)
N1—C12	1.4779 (17)	C23—H23	0.9500
N2—C21	1.3333 (15)	C24—H24A	0.9500
N2—C22	1.4738 (16)	C24—H24B	0.9500
N2—C25	1.4749 (16)	C25—C26	1.490 (2)
C12—C13	1.490 (2)	C25—H25A	0.9900
C12—H12A	0.9900	C25—H25B	0.9900
C12—H12B	0.9900	C26—C27	1.307 (2)
C13—C14	1.308 (2)	C26—H26	0.9500
C13—H13	0.9500	C27—H27A	0.9500
C14—H14A	0.9500	C27—H27B	0.9500
C14—H14B	0.9500		
S11—Cd1—S22	143.705 (13)	N1—C15—H15A	109.1
S11—Cd1—S12 ⁱ	103.129 (12)	C16—C15—H15A	109.1
S22—Cd1—S12 ⁱ	111.289 (11)	N1—C15—H15B	109.1
S11—Cd1—S21	108.203 (11)	C16—C15—H15B	109.1
S22—Cd1—S21	70.264 (10)	H15A—C15—H15B	107.8
S12 ⁱ —Cd1—S21	110.826 (11)	C17—C16—C15	124.89 (14)
S11—Cd1—S12	67.486 (10)	C17—C16—H16	117.6
S22—Cd1—S12	96.950 (10)	C15—C16—H16	117.6
S12 ⁱ —Cd1—S12	96.257 (9)	C16—C17—H17A	120.0
S21—Cd1—S12	152.651 (11)	C16—C17—H17B	120.0
C11—S11—Cd1	91.26 (4)	H17A—C17—H17B	120.0
C11—S12—Cd1 ⁱ	100.48 (4)	N2—C21—S21	120.81 (9)
C11—S12—Cd1	82.68 (4)	N2—C21—S22	119.72 (9)
Cd1 ⁱ —S12—Cd1	83.743 (9)	S21—C21—S22	119.47 (7)
C21—S21—Cd1	84.58 (4)	N2—C22—C23	112.57 (11)
C21—S22—Cd1	85.57 (4)	N2—C22—H22A	109.1
C11—N1—C15	123.59 (11)	C23—C22—H22A	109.1
C11—N1—C12	121.48 (11)	N2—C22—H22B	109.1
C15—N1—C12	114.93 (11)	C23—C22—H22B	109.1
C21—N2—C22	123.16 (10)	H22A—C22—H22B	107.8
C21—N2—C25	122.11 (11)	C24—C23—C22	123.46 (19)
C22—N2—C25	114.53 (10)	C24—C23—H23	118.3
N1—C11—S11	120.74 (10)	C22—C23—H23	118.3
N1—C11—S12	120.64 (10)	C23—C24—H24A	120.0
S11—C11—S12	118.58 (7)	C23—C24—H24B	120.0
N1—C12—C13	113.50 (11)	H24A—C24—H24B	120.0
N1—C12—H12A	108.9	N2—C25—C26	111.95 (11)
C13—C12—H12A	108.9	N2—C25—H25A	109.2
N1—C12—H12B	108.9	C26—C25—H25A	109.2
C13—C12—H12B	108.9	N2—C25—H25B	109.2
H12A—C12—H12B	107.7	C26—C25—H25B	109.2
C14—C13—C12	123.61 (16)	H25A—C25—H25B	107.9
C14—C13—H13	118.2	C27—C26—C25	123.99 (18)
C12—C13—H13	118.2	C27—C26—H26	118.0
C13—C14—H14A	120.0	C25—C26—H26	118.0

C13—C14—H14B	120.0	C26—C27—H27A	120.0
H14A—C14—H14B	120.0	C26—C27—H27B	120.0
N1—C15—C16	112.59 (12)	H27A—C27—H27B	120.0
C15—N1—C11—S11	−179.31 (10)	N1—C15—C16—C17	128.82 (17)
C12—N1—C11—S11	1.48 (17)	C22—N2—C21—S21	8.51 (17)
C15—N1—C11—S12	2.97 (17)	C25—N2—C21—S21	−176.94 (10)
C12—N1—C11—S12	−176.24 (9)	C22—N2—C21—S22	−171.47 (10)
Cd1—S11—C11—N1	−178.09 (10)	C25—N2—C21—S22	3.08 (17)
Cd1—S11—C11—S12	−0.33 (7)	Cd1—S21—C21—N2	−176.69 (10)
Cd1 ⁱ —S12—C11—N1	−99.72 (10)	Cd1—S21—C21—S22	3.29 (6)
Cd1—S12—C11—N1	178.07 (10)	Cd1—S22—C21—N2	176.65 (10)
Cd1 ⁱ —S12—C11—S11	82.51 (7)	Cd1—S22—C21—S21	−3.33 (7)
Cd1—S12—C11—S11	0.30 (6)	C21—N2—C22—C23	−114.38 (14)
C11—N1—C12—C13	−86.54 (16)	C25—N2—C22—C23	70.69 (16)
C15—N1—C12—C13	94.18 (15)	N2—C22—C23—C24	−123.84 (16)
N1—C12—C13—C14	−123.54 (16)	C21—N2—C25—C26	−91.28 (15)
C11—N1—C15—C16	110.28 (15)	C22—N2—C25—C26	83.71 (15)
C12—N1—C15—C16	−70.47 (16)	N2—C25—C26—C27	−122.19 (18)

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

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12B $\cdots$ S11	0.99	2.59	2.9783 (14)	103
C15—H15A $\cdots$ S12	0.99	2.50	3.0438 (14)	115
C22—H22B $\cdots$ S21	0.99	2.50	3.0381 (13)	114
C25—H25B $\cdots$ S22	0.99	2.56	2.9845 (14)	106