



# Crystal structure of *catena*-poly[[[bis(pyridine-4-carbothioamide- $\kappa N^1$ )cadmium]-di- $\mu$ -thiocyanato- $\kappa^2 N:S;\kappa^2 S:N$ ] methanol disolvate]

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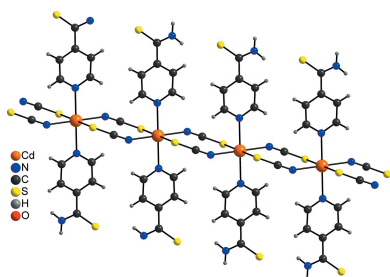
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The asymmetric unit of the polymeric title compound,  $\{[\text{Cd}(\text{NCS})_2(\text{C}_6\text{H}_6\text{N}_2\text{S})] \cdot 2\text{CH}_3\text{OH}\}_n$ , consists of one cadmium(II) cation that is located on a centre of inversion as well as one thiocyanate anion, one pyridine-4-carbothioamide ligand and one methanol molecule in general positions. The  $\text{Cd}^{\text{II}}$  cations are octahedrally coordinated by the pyridine N atom of two pyridine-4-carbothioamide ligands and by the S and N atoms of four thiocyanate anions and are linked into chains along [010] by pairs of anionic ligands. These chains are further linked into layers extending along (201) by intermolecular  $\text{N}-\text{H} \cdots \text{O}$  and  $\text{O}-\text{H} \cdots \text{S}$  hydrogen bonds. One of the amino H atoms of the pyridine-4-carbothioamide ligand is hydrogen-bonded to the O atom of a methanol molecule, and a symmetry-related methanol molecule is the donor group to the S atom of another pyridine-4-carbothioamide ligand whereby each of the pyridine-4-carbothioamide ligands forms two pairs of centrosymmetric  $\text{N}-\text{H} \cdots \text{S}$  and  $\text{O}-\text{H} \cdots \text{S}$  hydrogen bonds. The methanol molecules are equally disordered over two orientations.

## 1. Chemical context

Thiocyanato anions are versatile ligands that can coordinate to metal cations in different ways (Näther *et al.*, 2013). In this context, compounds in which paramagnetic metal cations are linked into chains by  $\mu$ -1,3 bridging anionic ligands are of special interest, because they can show different magnetic behavior (Palion-Gazda *et al.*, 2015). This is the case *e.g.* for compounds of general composition  $M(\text{NCS})_2(L)_2$  ( $M = \text{Mn}$ , Fe, Co and Ni;  $L =$  pyridine derivative) that frequently show cooperative magnetic properties like ferromagnetic or anti-ferromagnetic ordering or a slow relaxation of the magnetization indicative for single chain magnetic behavior (Näther *et al.*, 2013; Wöhlert *et al.*, 2011; Boeckmann & Näther, 2012; Werner *et al.*, 2015*a,b*). Unfortunately, compounds with a bridging coordination are frequently less stable than those in which these anionic ligands are only *N*-terminally coordinating. Hence, we have developed an alternative synthesis procedure which is based on thermal decomposition of suitable precursor compounds and leads directly to the formation of the desired compounds (Näther *et al.*, 2013). However, following this procedure only microcrystalline materials are obtained. This is the reason why we are also interested in the diamagnetic cadmium analogues. This metal cation is much more chalcophilic than most paramagnetic cations, which means that the desired compounds with a bridging coordination of the anionic ligands can easily be crystallized and characterized by single crystal X-ray diffrac-

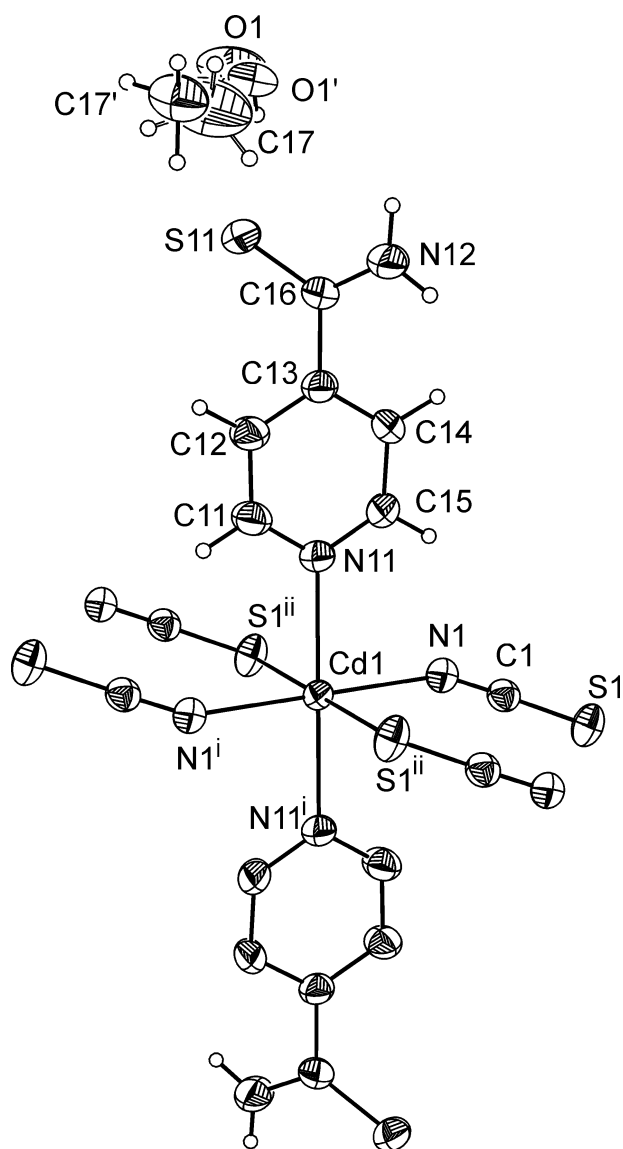


**Table 1**  
Selected bond lengths (Å).

Cd1–N1	2.3212 (18)	Cd1–S1 <sup>i</sup>	2.7174 (6)
Cd1–N11	2.3576 (18)		

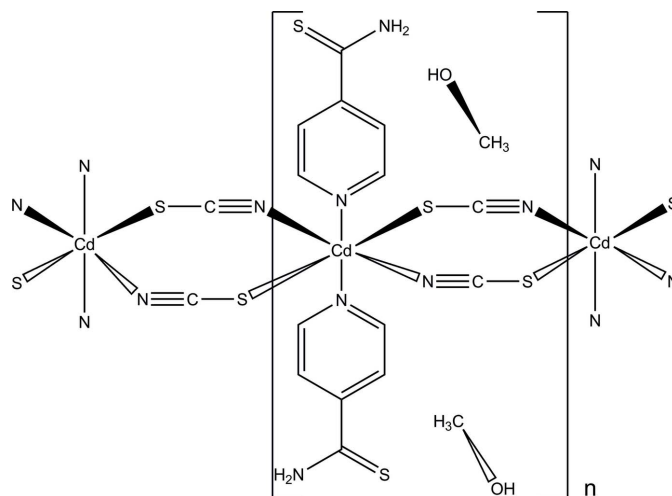
Symmetry code: (i)  $x, y - 1, z$ .

tion (Wöhlert *et al.*, 2013). In several cases, the resulting structures are isotopic to the paramagnetic analogues and therefore the latter can be refined by the Rietveld method using the crystallographic data of the respective Cd<sup>II</sup> compound (Wöhlert *et al.*, 2013). In the scope of our systematic work, we became interested in pyridine-4-carbo-



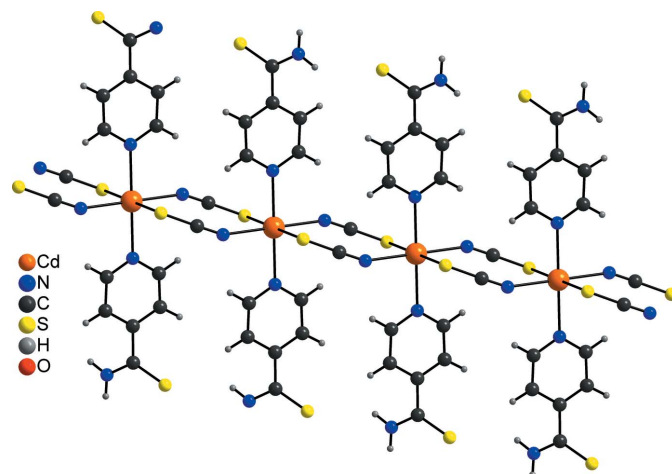
**Figure 1**  
The coordination of the Cd<sup>II</sup> cation in the structure of the title compound; the two orientations of the methanol solvent molecule are shown. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $x, y + 1, z$ ; (iii)  $-x + 1, -y + 2, -z + 1$ .]

thioamide as another ligand that was reacted with cadmium(II) thiocyanate to give the title compound.



## 2. Structural commentary

The asymmetric unit of the title compound,  $[\text{Cd}(\text{NCS})_2(\text{C}_6\text{H}_6\text{N}_2\text{S})] \cdot 2\text{CH}_3\text{OH}$ , consists of a Cd<sup>II</sup> cation that is located on a centre of inversion as well as one thiocyanato anion, one pyridine-4-carbothioamide ligand and one methanol molecule in general positions. The Cd<sup>II</sup> cation is sixfold coordinated by two N-bonding pyridinethioamide ligands as well as two N- and two S-coordinating thiocyanate anions in an all *trans* distorted octahedral environment (Fig. 1). As expected, the Cd–N bond length to the negatively charged thiocyanate anion is significantly shorter than to the pyridine-4-carbothioamide N atom; the Cd–S bond length is within the normal range (Table 1). The Cd<sup>II</sup> cations are linked by centrosymmetric pairs of anionic ligands into chains along [010] (Fig. 2). The methanol molecule is equally disordered over two orientations.



**Figure 2**  
View of a Cd–thiocyanate chain in the crystal structure of the title compound.

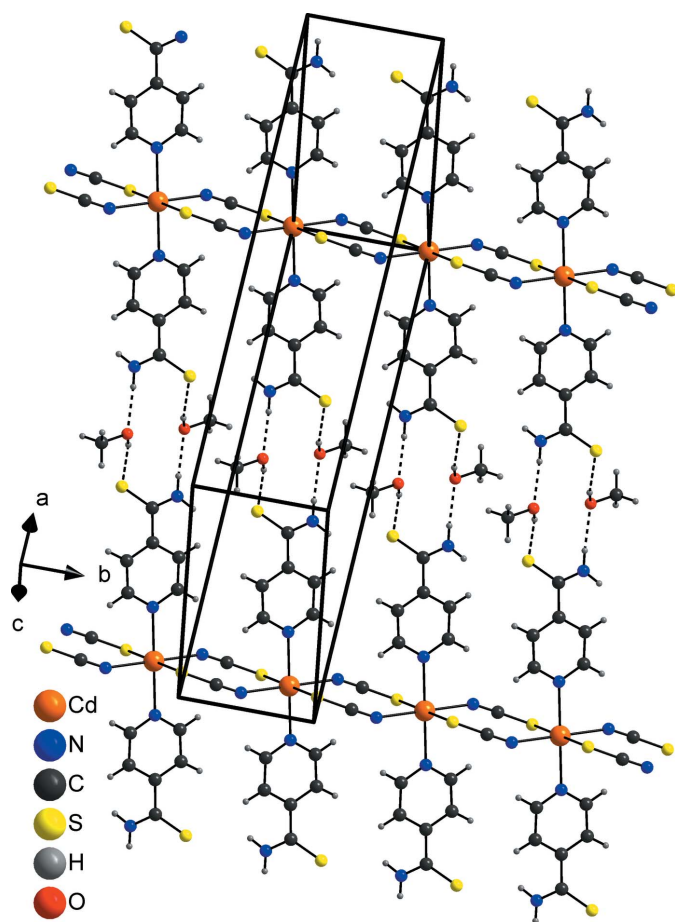
**Table 2**  
Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C11—H11···N1 <sup>ii</sup>	0.95	2.69	3.335 (3)	126
C12—H12···S1 <sup>iii</sup>	0.95	2.86	3.762 (2)	158
C15—H15···N1	0.95	2.54	3.230 (3)	130
N12—H12 <i>B</i> ···O1 <sup>iv</sup>	0.88	2.02	2.883 (10)	165
N12—H12 <i>B</i> ···O1 <sup>iv</sup>	0.88	1.88	2.740 (12)	165
N12—H12 <i>A</i> ···S1 <sup>v</sup>	0.88	2.90	3.560 (3)	133
N12—H12 <i>A</i> ···S11 <sup>vi</sup>	0.88	2.87	3.522 (2)	132
O1—H1···S11	0.84	2.53	3.351 (12)	165
O1'—H1'···S11	0.84	2.46	3.250 (12)	156

Symmetry codes: (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x, -y+1, z+\frac{1}{2}$ ; (iv)  $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$ ; (v)  $x, -y+2, z+\frac{1}{2}$ ; (vi)  $x, y+1, z$ .

### 3. Supramolecular features

In the crystal structure, the neutral chains are linked into layers extending along (201) by intermolecular N—H···O and O—H···S hydrogen bonding *via* the methanol solvent molecules (Fig. 3). Each pyridine-4-carbothioamide ligand of neighbouring chains makes one N—H···O hydrogen bond to the hydroxyl O atom that acts as an acceptor, and one O—



**Figure 3**  
View of one layer in the crystal structure of the title compound with hydrogen bonds shown as dashed lines. Only one orientation of the disordered methanol molecule is shown.

**Table 3**  
Experimental details.

Crystal data	
Chemical formula	[Cd(NCS) <sub>2</sub> (C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> S)]·2CH <sub>4</sub> O
<i>M<sub>r</sub></i>	1138.04
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	200
<i>a</i> , <i>b</i> , <i>c</i> (Å)	25.1891 (10), 5.8729 (2), 15.5080 (6)
$\beta$ (°)	90.124 (3)
<i>V</i> (Å <sup>3</sup> )	2294.14 (15)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.34
Crystal size (mm)	0.18 × 0.14 × 0.10
Data collection	
Diffractometer	Stoe <i>IPDS2</i>
Absorption correction	Numerical ( <i>X-SHAPE</i> and <i>X-RED32</i> ; Stoe, 2008)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.644, 0.800
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	15896, 2515, 2208
<i>R<sub>int</sub></i>	0.032
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.639
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.026, 0.067, 1.06
No. of reflections	2515
No. of parameters	156
No. of restraints	37
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.41, -0.47

Computer programs: *X-AREA* (Stoe, 2008), *SHELXS97* and *XP* in *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999) and *publCIF* (Westrip, 2010).

H···S hydrogen bond between the hydroxyl H atom and the S atom of the pyridine-4-carbothioamide ligand (Fig. 3 and Table 2). The hydrogen-bonding geometry is very similar for the two disordered and slightly differently oriented methanol molecules (Table 2). This arrangement leads to 12-membered rings [graph-set notation *R*<sub>4</sub><sup>4</sup>(12); Etter *et al.*, 1990] in which four donor and four acceptors are involved (Fig. 2 and Table 2). There are additional C—H···N, C—H···S and N—H···S interactions of much weaker nature that consolidate the three-dimensional network (Table 2).

### 4. Database survey

According to the Cambridge Structural Database (Version 5.36, last update 2015; Groom & Allen, 2014) no coordination compounds with pyridine-4-carbothioamide have been structurally characterized. There is only one crystal structure of the ligand itself reported at room temperature and at 100 K (Colleter & Gadret, 1967; Eccles *et al.*, 2014). The crystal structure of the protonated ligand 4-thiocarbamoylpyridinium iodide was also reported recently (Shotonwa & Boéré, 2014).

### 5. Synthesis and crystallization

CdSO<sub>4</sub>·3/8H<sub>2</sub>O was purchased from Merck and pyridine-4-carbothioamide and Ba(NCS)<sub>2</sub>·3H<sub>2</sub>O were purchased from Alfa Aesar. Cd(NCS)<sub>2</sub> was synthesized by stirring 17.5 g

(57.0 mmol)  $\text{Ba}(\text{NCS})_2 \cdot 3\text{H}_2\text{O}$  and 14.6 g (57.0 mmol)  $\text{CdSO}_4 \cdot 3/8\text{H}_2\text{O}$  in 300 ml water at room temperature for 3 h. The white residue of  $\text{BaSO}_4$  was filtered off and the resulting solution dried at 353 K. The homogeneity of the product was checked by X-ray powder diffraction and elemental analysis. The title compound was obtained by reaction of 11.4 mg  $\text{Cd}(\text{NCS})_2$  (0.05 mmol) with 27.6 mg pyridine-4-carbothioamide (0.2 mmol) in boiling methanol (2 ml). Crystals suitable for single-crystal x-ray diffraction formed after cooling.

## 6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. The C—H, O—H and N—H hydrogen atoms were located in a difference map but were positioned with idealized geometry (methyl and O—H hydrogen atoms allowed to rotate but not to tip) and were refined with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  (1.5 for methyl and O—H hydrogen atoms) using a riding model with C—H = 0.95 Å for aromatic, C—H = 0.98 Å for methyl, N—H = 0.88 Å and O—H = 0.84 Å, respectively. The methanol molecule is equally disordered over two orientations and was refined using a split model using SAME restraints (Sheldrick, 2015).

## Acknowledgements

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## supporting information

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## Crystal structure of *catena*-poly[[[bis(pyridine-4-carbothioamide- $\kappa$ N<sup>1</sup>)cadmium]-di- $\mu$ -thiocyanato- $\kappa^2$ N:S; $\kappa^2$ S:N] methanol disolvate]

Tristan Neumann, Inke Jess and Christian Näther

### Computing details

Data collection: *X-AREA* (Stoe, 2008); cell refinement: *X-AREA* (Stoe, 2008); data reduction: *X-AREA* (Stoe, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *publCIF* (Westrip, 2010).

*catena*-Poly[[[bis(pyridine-4-carbothioamide- $\kappa$ N<sup>1</sup>)cadmium]-di- $\mu$ -thiocyanato- $\kappa^2$ N:S; $\kappa^2$ S:N] methanol disolvate]

### Crystal data

[Cd(NCS)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>S)]·2CH<sub>4</sub>O

*M<sub>r</sub>* = 1138.04

Monoclinic, *C2/c*

*a* = 25.1891 (10) Å

*b* = 5.8729 (2) Å

*c* = 15.5080 (6) Å

$\beta$  = 90.124 (3)°

*V* = 2294.14 (15) Å<sup>3</sup>

*Z* = 2

*F*(000) = 1144

*D<sub>x</sub>* = 1.647 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 16834 reflections

$\theta$  = 1.3–27°

$\mu$  = 1.34 mm<sup>-1</sup>

*T* = 200 K

Block, colorless

0.18 × 0.14 × 0.10 mm

### Data collection

Stoe IPDS-2  
diffractometer

$\omega$  scans

Absorption correction: numerical  
(*X-SHAPE* and *X-RED32*; Stoe, 2008)

*T<sub>min</sub>* = 0.644, *T<sub>max</sub>* = 0.800

15896 measured reflections

2515 independent reflections

2208 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.032

$\theta_{\max}$  = 27.0°,  $\theta_{\min}$  = 1.6°

*h* = -32→32

*k* = -7→7

*l* = -19→19

### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.026

*wR*(*F*<sup>2</sup>) = 0.067

*S* = 1.06

2515 reflections

156 parameters

37 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

*w* = 1/[ $\sigma^2(F_o^2) + (0.0471P)^2$ ]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

( $\Delta/\sigma$ )<sub>max</sub> < 0.001

$\Delta\rho_{\max}$  = 0.41 e Å<sup>-3</sup>

$\Delta\rho_{\min}$  = -0.47 e Å<sup>-3</sup>

Extinction correction: *SHELXL2014* (Sheldrick,  
2015), *F<sub>c</sub>*\* = *kF<sub>c</sub>*[1 + 0.001*xF<sub>c</sub>*<sup>2</sup> $\lambda^3/\sin(2\theta)$ ]<sup>-1/4</sup>

Extinction coefficient: 0.0015 (2)

*Special details*

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cd1	0.5000	0.5000	0.5000	0.02964 (10)	
N1	0.45141 (7)	0.8201 (3)	0.46141 (12)	0.0363 (4)	
C1	0.44617 (9)	1.0011 (3)	0.43255 (13)	0.0317 (4)	
S1	0.43930 (2)	1.25424 (10)	0.38878 (4)	0.04069 (15)	
N11	0.43968 (8)	0.4286 (3)	0.61284 (12)	0.0361 (4)	
C11	0.44093 (9)	0.2407 (4)	0.66130 (15)	0.0426 (5)	
H11	0.4684	0.1332	0.6514	0.051*	
C12	0.40419 (9)	0.1946 (4)	0.72524 (14)	0.0405 (5)	
H12	0.4060	0.0563	0.7569	0.049*	
C13	0.36515 (9)	0.3512 (4)	0.74238 (13)	0.0353 (5)	
C14	0.36407 (12)	0.5485 (4)	0.6943 (2)	0.0542 (7)	
H14	0.3381	0.6623	0.7050	0.065*	
C15	0.40177 (12)	0.5776 (5)	0.62990 (18)	0.0532 (7)	
H15	0.4002	0.7124	0.5962	0.064*	
C16	0.32407 (9)	0.3067 (4)	0.81005 (14)	0.0366 (5)	
N12	0.31373 (11)	0.4768 (4)	0.86169 (16)	0.0540 (6)	
H12A	0.3305	0.6070	0.8554	0.065*	
H12B	0.2900	0.4610	0.9028	0.065*	
S11	0.29342 (3)	0.05620 (11)	0.81316 (4)	0.04527 (16)	
O1	0.2777 (4)	0.0596 (16)	1.0276 (8)	0.067 (3)	0.5
H1	0.2760	0.0718	0.9737	0.100*	0.5
C17	0.3143 (5)	-0.101 (3)	1.0489 (13)	0.062 (3)	0.5
H17A	0.3476	-0.0703	1.0185	0.093*	0.5
H17B	0.3010	-0.2520	1.0324	0.093*	0.5
H17C	0.3206	-0.0978	1.1113	0.093*	0.5
O1'	0.2639 (4)	-0.0102 (19)	1.0155 (8)	0.079 (3)	0.5
H1'	0.2637	0.0358	0.9642	0.118*	0.5
C17'	0.3144 (8)	-0.019 (4)	1.0447 (17)	0.113 (8)	0.5
H17D	0.3348	0.1072	1.0201	0.169*	0.5
H17E	0.3306	-0.1640	1.0274	0.169*	0.5
H17F	0.3146	-0.0074	1.1077	0.169*	0.5

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.03369 (13)	0.02444 (13)	0.03081 (13)	-0.00052 (8)	0.00757 (8)	0.00137 (8)
N1	0.0362 (9)	0.0302 (10)	0.0427 (10)	0.0018 (7)	0.0035 (8)	0.0034 (8)
C1	0.0325 (10)	0.0329 (11)	0.0298 (9)	-0.0004 (8)	0.0016 (8)	-0.0038 (8)
S1	0.0504 (3)	0.0295 (3)	0.0421 (3)	-0.0022 (2)	-0.0116 (2)	0.0059 (2)



N11	0.0383 (10)	0.0333 (9)	0.0366 (9)	-0.0026 (8)	0.0111 (8)	0.0000 (8)
C11	0.0392 (12)	0.0483 (13)	0.0404 (11)	0.0086 (10)	0.0107 (9)	0.0094 (10)
C12	0.0404 (12)	0.0444 (13)	0.0368 (11)	0.0058 (10)	0.0090 (9)	0.0105 (10)
C13	0.0377 (11)	0.0342 (11)	0.0341 (10)	-0.0052 (9)	0.0090 (9)	-0.0034 (8)
C14	0.0611 (16)	0.0340 (12)	0.0677 (17)	0.0117 (11)	0.0367 (14)	0.0063 (12)
C15	0.0667 (17)	0.0303 (11)	0.0628 (16)	0.0054 (12)	0.0336 (14)	0.0104 (11)
C16	0.0364 (11)	0.0380 (11)	0.0353 (10)	0.0017 (9)	0.0096 (9)	0.0005 (9)
N12	0.0645 (15)	0.0432 (12)	0.0543 (13)	-0.0078 (10)	0.0297 (11)	-0.0077 (10)
S11	0.0490 (3)	0.0376 (3)	0.0493 (3)	-0.0070 (3)	0.0158 (3)	0.0009 (3)
O1	0.066 (6)	0.063 (4)	0.072 (6)	0.006 (3)	0.043 (5)	0.005 (3)
C17	0.045 (5)	0.091 (7)	0.050 (5)	0.008 (4)	-0.004 (3)	0.005 (5)
O1'	0.059 (5)	0.127 (10)	0.050 (3)	0.006 (5)	0.019 (3)	0.019 (5)
C17'	0.084 (10)	0.18 (2)	0.077 (10)	0.001 (11)	0.003 (7)	-0.013 (12)

*Geometric parameters (Å, °)*

Cd1—N1 <sup>i</sup>	2.3212 (18)	C14—C15	1.390 (3)
Cd1—N1	2.3212 (18)	C14—H14	0.9500
Cd1—N11 <sup>i</sup>	2.3575 (18)	C15—H15	0.9500
Cd1—N11	2.3576 (18)	C16—N12	1.307 (3)
Cd1—S1 <sup>ii</sup>	2.7174 (6)	C16—S11	1.662 (2)
Cd1—S1 <sup>iii</sup>	2.7174 (6)	N12—H12A	0.8800
N1—C1	1.161 (3)	N12—H12B	0.8800
C1—S1	1.643 (2)	O1—C17	1.361 (13)
S1—Cd1 <sup>iv</sup>	2.7174 (6)	O1—H1	0.8400
N11—C15	1.322 (3)	C17—H17A	0.9800
N11—C11	1.335 (3)	C17—H17B	0.9800
C11—C12	1.385 (3)	C17—H17C	0.9800
C11—H11	0.9500	O1'—C17'	1.351 (15)
C12—C13	1.373 (3)	O1'—H1'	0.8400
C12—H12	0.9500	C17'—H17D	0.9800
C13—C14	1.378 (3)	C17'—H17E	0.9800
C13—C16	1.498 (3)	C17'—H17F	0.9800
N1 <sup>i</sup> —Cd1—N1	180.00 (9)	C12—C13—C16	121.0 (2)
N1 <sup>i</sup> —Cd1—N11 <sup>i</sup>	89.72 (7)	C14—C13—C16	120.8 (2)
N1—Cd1—N11 <sup>i</sup>	90.28 (7)	C13—C14—C15	118.6 (2)
N1 <sup>i</sup> —Cd1—N11	90.28 (7)	C13—C14—H14	120.7
N1—Cd1—N11	89.72 (7)	C15—C14—H14	120.7
N11 <sup>i</sup> —Cd1—N11	180.0	N11—C15—C14	123.9 (2)
N1 <sup>i</sup> —Cd1—S1 <sup>ii</sup>	91.67 (5)	N11—C15—H15	118.1
N1—Cd1—S1 <sup>ii</sup>	88.33 (5)	C14—C15—H15	118.1
N11 <sup>i</sup> —Cd1—S1 <sup>ii</sup>	89.20 (5)	N12—C16—C13	115.8 (2)
N11—Cd1—S1 <sup>ii</sup>	90.80 (5)	N12—C16—S11	124.43 (17)
N1 <sup>i</sup> —Cd1—S1 <sup>iii</sup>	88.33 (5)	C13—C16—S11	119.74 (16)
N1—Cd1—S1 <sup>iii</sup>	91.67 (5)	C16—N12—H12A	120.0
N11 <sup>i</sup> —Cd1—S1 <sup>iii</sup>	90.80 (5)	C16—N12—H12B	120.0
N11—Cd1—S1 <sup>iii</sup>	89.20 (5)	H12A—N12—H12B	120.0

S1 <sup>ii</sup> —Cd1—S1 <sup>iii</sup>	180.0	C17—O1—H1	109.5
C1—N1—Cd1	154.23 (17)	O1—C17—H17A	109.5
N1—C1—S1	178.2 (2)	O1—C17—H17B	109.5
C1—S1—Cd1 <sup>iv</sup>	99.19 (7)	H17A—C17—H17B	109.5
C15—N11—C11	116.8 (2)	O1—C17—H17C	109.5
C15—N11—Cd1	119.86 (16)	H17A—C17—H17C	109.5
C11—N11—Cd1	123.37 (15)	H17B—C17—H17C	109.5
N11—C11—C12	123.3 (2)	C17'—O1'—H1'	109.5
N11—C11—H11	118.3	O1'—C17'—H17D	109.5
C12—C11—H11	118.3	O1'—C17'—H17E	109.5
C13—C12—C11	119.2 (2)	H17D—C17'—H17E	109.5
C13—C12—H12	120.4	O1'—C17'—H17F	109.5
C11—C12—H12	120.4	H17D—C17'—H17F	109.5
C12—C13—C14	118.2 (2)	H17E—C17'—H17F	109.5

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (ii)  $x, y-1, z$ ; (iii)  $-x+1, -y+2, -z+1$ ; (iv)  $x, y+1, z$ .

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

<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>
C11—H11 $\cdots$ N1 <sup>i</sup>	0.95	2.69	3.335 (3)	126
C12—H12 $\cdots$ S1 <sup>v</sup>	0.95	2.86	3.762 (2)	158
C15—H15 $\cdots$ N1	0.95	2.54	3.230 (3)	130
N12—H12B $\cdots$ O1 <sup>vi</sup>	0.88	2.02	2.883 (10)	165
N12—H12B $\cdots$ O1' <sup>vi</sup>	0.88	1.88	2.740 (12)	165
N12—H12A $\cdots$ S1 <sup>vii</sup>	0.88	2.90	3.560 (3)	133
N12—H12A $\cdots$ S11 <sup>iv</sup>	0.88	2.87	3.522 (2)	132
O1—H1 $\cdots$ S11	0.84	2.53	3.351 (12)	165
O1'—H1' $\cdots$ S11	0.84	2.46	3.250 (12)	156

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (iv)  $x, y+1, z$ ; (v)  $x, -y+1, z+1/2$ ; (vi)  $-x+1/2, -y+1/2, -z+2$ ; (vii)  $x, -y+2, z+1/2$ .