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catena-Poly[[bis(2-methoxyaniline- κ N)-cadmium]-di- μ -thiocyanato- κ^2 N:S; κ^2 S:N]

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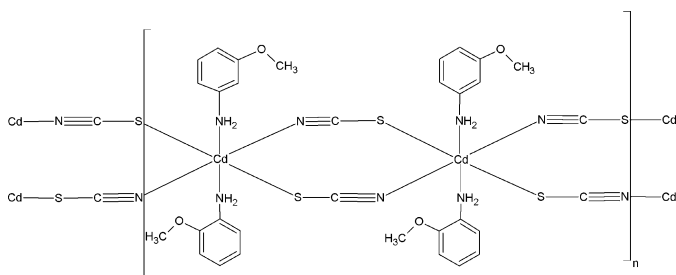
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Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.025; wR factor = 0.055; data-to-parameter ratio = 18.5.

The structure of the title compound, $[\text{Cd}(\text{NCS})_2(\text{C}_7\text{H}_9\text{NO})_2]_n$, consists of cadmium–thiocyanate layers parallel to the ab plane. Pairs of Cd^{II} ions are bridged by two end-to-end inversely bridging μ -NCS- $N:S$ thiocyanate groups, forming a two-dimensional network with the remaining two *trans* positions of the octahedrally coordinated Cd^{II} ions occupied by the N atoms of two neutral 2-methoxyaniline ligands. The crystal structure is stabilized by intralayer $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds.

Related literature

For related structures, see: Wöhlert *et al.* (2012, 2013); Bai *et al.* (2011); Yang *et al.* (2001). For HSCN synthesis, see: Bartlett *et al.* (1969). For the effects of substituents on the internal angles of the benzene ring, see: Domenicano & Murray-Rust (1979). For non-linear optical and luminescence properties of related compounds, see: Chen *et al.* (2000); Bai *et al.* (2011). For electric and dielectric properties of related compounds, see: Karoui *et al.* (2013).



Experimental

Crystal data

$[\text{Cd}(\text{NCS})_2(\text{C}_7\text{H}_9\text{NO})_2]$
 $M_r = 474.89$
 Orthorhombic, $Pbca$
 $a = 6.6860$ (2) Å
 $b = 23.3658$ (7) Å
 $c = 24.3281$ (8) Å
 $V = 3800.6$ (2) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.39$ mm⁻¹
 $T = 150$ K
 $0.33 \times 0.18 \times 0.11$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2011)
 $T_{\text{min}} = 0.741$, $T_{\text{max}} = 0.859$
 16897 measured reflections
 4210 independent reflections
 3262 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.055$
 $S = 1.02$
 4210 reflections
 228 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Table 1
Selected bond lengths (Å).

Cd1—N2	2.2724 (19)	Cd1—N21	2.3718 (17)
Cd1—N1	2.3142 (18)	Cd1—S1 ⁱ	2.7306 (6)
Cd1—N11	2.3653 (17)	Cd1—S2 ⁱⁱ	2.7449 (6)

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

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

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N11}-\text{H11A}\cdots\text{S2}^{\text{iii}}$	0.92	2.50	3.4182 (17)	174
$\text{N21}-\text{H21B}\cdots\text{S1}^{\text{iv}}$	0.92	2.66	3.5637 (18)	169

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

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2011); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Berndt, 2001) and Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: WinGX (Farrugia, 2012) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5058).

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supporting information

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catena-Poly[[bis(2-methoxyaniline- κ N)cadmium]-di- μ -thiocyanato- κ^2 N:S; κ^2 S:N]

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S1. Comment

The crystal engineering of inorganic-organic hybrid coordination polymers is currently one of the most active fields in coordination chemistry, supramolecular and materials chemistry. These compounds attract significant attention for their architectures and topologies (Yang *et al.*, 2001). Hybrid inorganic-organic thiocyanate materials exhibit interesting physical properties such electrical conductivity and dielectric relaxation process (Karoui *et al.*, 2013) and may have potential applications in non-linear optics and luminescence (Chen *et al.*, 2000; Bai *et al.*, 2011). Herein we report the structure of a new polymeric hybrid title compound

As shown in Fig. 1, each cadmium atom, which sits on general position, is coordinated by two *trans* N-bonded and two *trans* S-bonded thiocyanato anions. Two *trans*-coordinated 2-methoxy aniline ligands complete the octahedral coordination geometry around cadmium. The crystal structure of the title compound consists of both simply and doubly μ -1,3-SCN-bridged two dimensional networks parallel to the *ab* plane with terminal neutral 2-methoxyaniline ligands (Fig. 2). In the CdN_4S_2 core, the Cd—N and Cd—S bonds span the range 2.2724 (19)–2.3718 (17) Å and 2.7306 (6)–2.7449 (6) Å, respectively (Table 1). These values are in good agreement with those observed in other similar complexes (Wöhlert *et al.*, 2012, 2013; Yang *et al.*, 2001). The bond angles involving the cadmium(II) cation range from 84.29 (6) to 95.50 (7)° and from 174.91 (2) to 175.76 (6)°. The double-bridging role of S1/C1/N1 anions gives rise to eight-membered $\text{Cd}_2(\text{SCN})_2$ rings in a chair conformation because of the almost linear SCN groups (S1–C1–N1 angle = 178.76 (21)°). The distance between adjacent Cd atoms in the $\text{Cd}_2(\text{SCN})_2$ rings is 5.9127 (4) Å. Again, these rings built up a 2-D sheet through their corner-sharing action at the two cadmium atoms *via* the linear S2/C2/N2 anions (S1–C1–N1 angle = 177.96 (21)°) and give rise to thirty-membered $[\text{Cd}_6(\mu\text{-SCN-N,S})_8]$ macrocycles as subunits, as shown in Fig. 2. The bond angles in the phenyl groups deviate significantly from the idealized value of 120° due to the effect of the substituent. In fact, it was established that the angular deformations of phenyl groups can be described as a sum of the effects of the different substituents (Domenicano & Murray-Rust, 1979). The phenyl rings of both independent 2-methoxyaniline ligands are planar with the greatest deviation from the six-atoms least-square plane of 0.0029 Å and 0.0073 Å. They are well ordered with C–C–C angles in agreement with the expected sp^2 hybridation. The π - π interactions between phenyl rings may be neglected (>4 Å); in fact the shortest distances between the centroids of the rings are: $\text{Cg1} \cdots \text{Cg1}^i = 5.6130$ (14) Å; $\text{Cg1} \cdots \text{Cg2}^{ii} = 5.5949$ (14) Å (Cg1 and Cg2 are the centroids of the C12–C17 and C22–C27 rings, respectively; symmetry codes: (i) $-0.5+x, +y, 1.5-z$; 2. $-x, -y, 1.-z$). The major contributions to the cohesion and the stability of the polymeric structure is the presence of intralayer N—H \cdots S hydrogen bonds which include two relatively long contacts, with H \cdots S and N \cdots S distances ranging from 2.50 to 2.66 Å and 3.4182 (17) Å to 3.5637 (18) Å, respectively (Table 2).

S2. Experimental

To 25 ml of an aqueous solution of thiocyanic acid (0.8 M) prepared using the published procedure (Bartlett *et al.*, 1969) an appropriate amount of cadmium carbonate (1.664 g, 10 mmol) was added and refluxed for 3 h. After cooling, 25 ml of methanol and 2.3 ml of a solution of 2-methoxyaniline (8.64 M) was added. The resulting solution was heated under reflux for 1 h and left to stand at ambient temperature. Well shaped colourless crystals were obtained after 2 h on slow evaporation of the solvent. They were washed with diethyl ether and dried over P_2O_5 .

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–0.98 Å, N—H = 0.92 Å, and with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

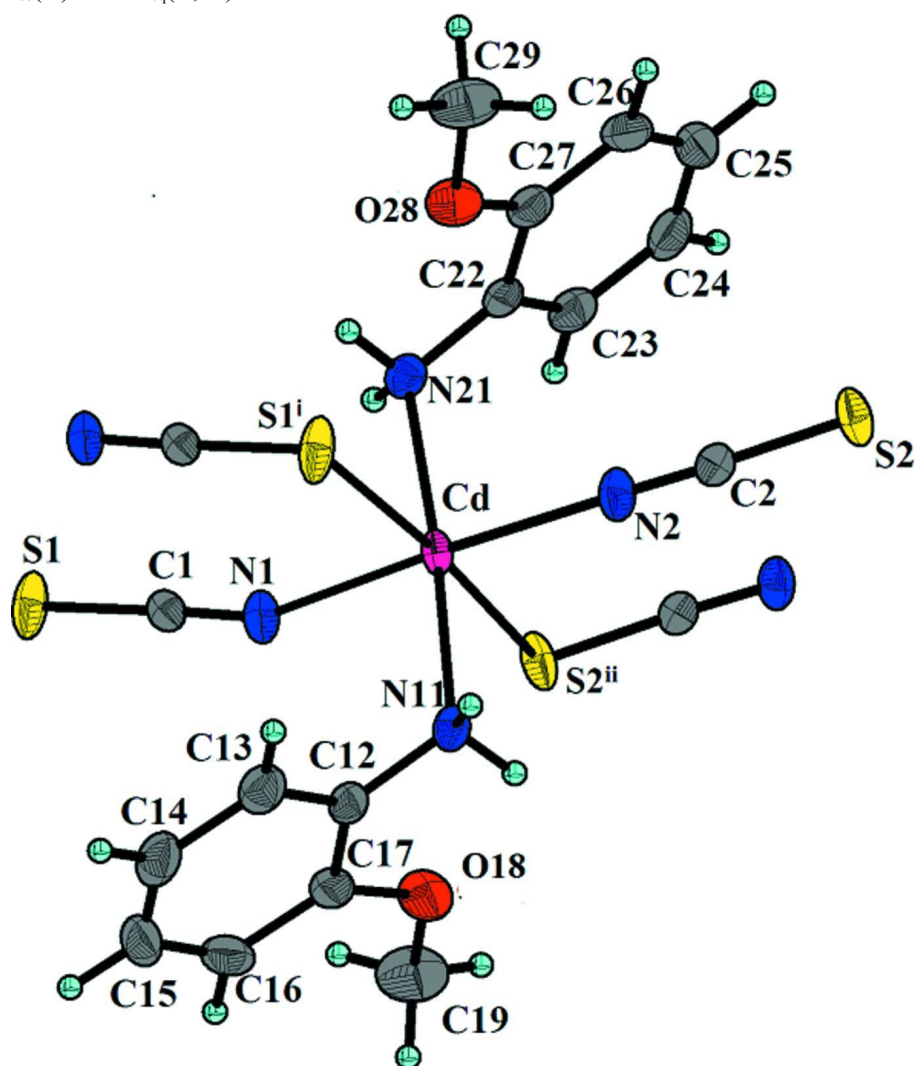


Figure 1

Crystal structure of the title compound, showing the coordination around the Cd^{2+} cation with displacement ellipsoids drawn at the 50% probability level.

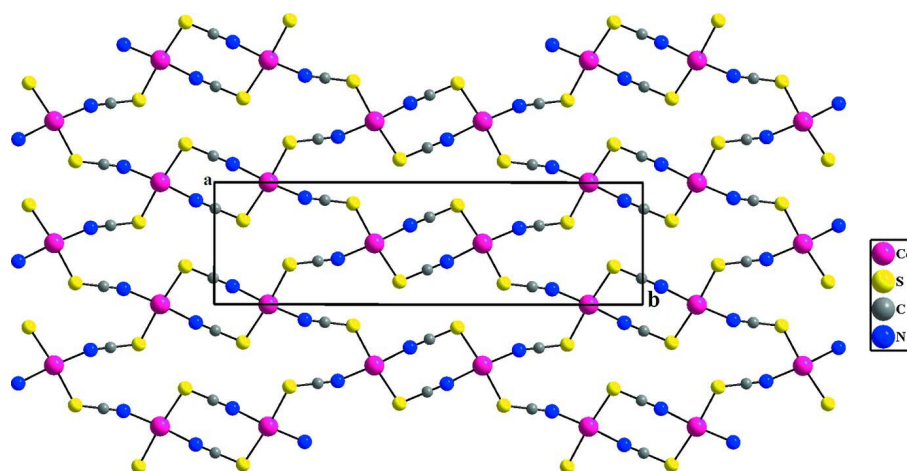


Figure 2

View at $z=0$ of the two-dimensional layer structure of the inorganic coordination polymer parallel to the ab plane. The organic ligands are omitted for clarity.

catena-Poly[[bis(2-methoxyaniline- κ N)cadmium]-di- μ -thiocyanato- κ^2 N:S; κ^2 S:N]

Crystal data

[Cd(NCS)₂(C₇H₉NO)₂]

$M_r = 474.89$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 6.6860$ (2) Å

$b = 23.3658$ (7) Å

$c = 24.3281$ (8) Å

$V = 3800.6$ (2) Å³

$Z = 8$

$F(000) = 1904$

$D_x = 1.660$ Mg m⁻³

$D_m = 1.593$ Mg m⁻³

D_m measured by flotation

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

Cell parameters from 5155 reflections

$\theta = 3.1$ – 27.4°

$\mu = 1.39$ mm⁻¹

$T = 150$ K

Prism, colourless

$0.33 \times 0.18 \times 0.11$ mm

Data collection

Bruker APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

CCD rotation images, thin slices scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2011)

$T_{\min} = 0.741$, $T_{\max} = 0.859$

16897 measured reflections

4210 independent reflections

3262 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -8 \rightarrow 8$

$k = -29 \rightarrow 30$

$l = -31 \rightarrow 20$

2 standard reflections every 120 min

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.055$

$S = 1.02$

4210 reflections

228 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

$$w = 1/[\sigma^2(F_o^2) + (0.0184P)^2 + 1.4548P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.004$

$$\Delta\rho_{\max} = 0.35 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$$

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.

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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.99993 (2)	0.126200 (7)	0.508711 (7)	0.02024 (6)
S1	0.68873 (8)	-0.06757 (2)	0.53717 (3)	0.03279 (16)
C1	0.7845 (3)	-0.00256 (9)	0.53832 (8)	0.0191 (5)
N1	0.8515 (3)	0.04293 (8)	0.54015 (8)	0.0253 (4)
S2	1.17331 (8)	0.32408 (2)	0.44237 (3)	0.02739 (14)
N2	1.1259 (3)	0.21155 (8)	0.48030 (8)	0.0266 (4)
C2	1.1461 (3)	0.25807 (9)	0.46565 (9)	0.0193 (5)
N11	1.1959 (2)	0.13518 (7)	0.58919 (7)	0.0213 (4)
H11A	1.3247	0.1440	0.5789	0.026*
H11B	1.1478	0.1657	0.6092	0.026*
C12	1.2028 (3)	0.08631 (9)	0.62450 (9)	0.0220 (5)
C13	1.3485 (3)	0.04507 (10)	0.61900 (10)	0.0312 (6)
H13	1.4520	0.0498	0.5926	0.037*
C14	1.3446 (4)	-0.00363 (11)	0.65207 (11)	0.0412 (7)
H14	1.4466	-0.0317	0.6488	0.049*
C15	1.1926 (5)	-0.01091 (11)	0.68948 (11)	0.0441 (7)
H15	1.1889	-0.0445	0.7115	0.053*
C16	1.0444 (4)	0.03030 (12)	0.69545 (9)	0.0362 (6)
H16	0.9394	0.0249	0.7213	0.043*
C17	1.0510 (3)	0.07931 (10)	0.66349 (9)	0.0258 (5)
O18	0.9195 (2)	0.12405 (7)	0.66597 (7)	0.0344 (4)
C19	0.7522 (4)	0.11868 (13)	0.70215 (11)	0.0478 (8)
H19A	0.6797	0.0833	0.6938	0.072*
H19B	0.6628	0.1515	0.6972	0.072*
H19C	0.7994	0.1176	0.7403	0.072*
N21	0.8084 (3)	0.10925 (8)	0.42829 (7)	0.0240 (4)
H21A	0.8731	0.0813	0.4085	0.029*
H21B	0.6879	0.0941	0.4393	0.029*
C22	0.7653 (3)	0.15518 (10)	0.39121 (9)	0.0230 (5)
C23	0.5968 (3)	0.18854 (10)	0.39643 (9)	0.0281 (5)
H23	0.5026	0.1805	0.4246	0.034*
C24	0.5637 (4)	0.23401 (11)	0.36050 (10)	0.0344 (6)

H24	0.4466	0.2568	0.3640	0.041*
C25	0.7010 (4)	0.24592 (11)	0.31981 (10)	0.0380 (6)
H25	0.6786	0.2771	0.2955	0.046*
C26	0.8727 (4)	0.21251 (11)	0.31418 (9)	0.0346 (6)
H26	0.9674	0.2209	0.2862	0.042*
C27	0.9044 (3)	0.16704 (10)	0.34953 (9)	0.0269 (5)
O28	1.0642 (2)	0.13068 (7)	0.34823 (7)	0.0348 (4)
C29	1.1988 (4)	0.13507 (13)	0.30289 (10)	0.0446 (7)
H29A	1.1241	0.1312	0.2684	0.067*
H29B	1.2992	0.1046	0.3053	0.067*
H29C	1.2655	0.1724	0.3038	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02022 (9)	0.01308 (9)	0.02743 (10)	-0.00211 (6)	0.00012 (7)	0.00258 (7)
S1	0.0237 (3)	0.0153 (3)	0.0594 (4)	-0.0043 (2)	0.0168 (3)	-0.0044 (3)
C1	0.0164 (9)	0.0193 (12)	0.0217 (11)	0.0047 (9)	0.0036 (9)	0.0024 (10)
N1	0.0238 (9)	0.0161 (10)	0.0361 (11)	0.0001 (8)	0.0062 (9)	0.0016 (9)
S2	0.0211 (3)	0.0175 (3)	0.0435 (3)	-0.0045 (2)	-0.0093 (3)	0.0096 (3)
N2	0.0265 (10)	0.0169 (10)	0.0364 (11)	-0.0047 (8)	0.0035 (9)	0.0010 (9)
C2	0.0143 (9)	0.0202 (12)	0.0235 (11)	-0.0014 (9)	-0.0001 (9)	-0.0028 (10)
N11	0.0192 (8)	0.0177 (10)	0.0272 (10)	-0.0018 (8)	0.0048 (8)	-0.0019 (8)
C12	0.0241 (10)	0.0196 (11)	0.0224 (11)	-0.0026 (9)	-0.0044 (9)	-0.0025 (10)
C13	0.0339 (12)	0.0283 (13)	0.0314 (13)	0.0025 (11)	-0.0080 (11)	-0.0051 (12)
C14	0.0588 (17)	0.0254 (14)	0.0392 (15)	0.0107 (13)	-0.0238 (14)	-0.0068 (13)
C15	0.077 (2)	0.0220 (14)	0.0334 (15)	-0.0083 (14)	-0.0267 (15)	0.0048 (12)
C16	0.0501 (15)	0.0380 (16)	0.0205 (12)	-0.0184 (13)	-0.0058 (11)	0.0031 (12)
C17	0.0309 (11)	0.0254 (13)	0.0211 (11)	-0.0053 (10)	-0.0024 (10)	-0.0010 (11)
O18	0.0304 (8)	0.0399 (11)	0.0330 (9)	0.0006 (8)	0.0131 (8)	0.0038 (8)
C19	0.0336 (14)	0.070 (2)	0.0400 (16)	-0.0100 (14)	0.0149 (12)	-0.0017 (16)
N21	0.0248 (9)	0.0219 (10)	0.0253 (10)	-0.0043 (8)	0.0037 (8)	-0.0030 (9)
C22	0.0289 (11)	0.0201 (12)	0.0201 (11)	-0.0065 (10)	-0.0032 (9)	-0.0052 (10)
C23	0.0294 (12)	0.0292 (13)	0.0259 (12)	-0.0053 (11)	-0.0023 (10)	-0.0073 (11)
C24	0.0422 (13)	0.0243 (13)	0.0366 (14)	0.0016 (12)	-0.0112 (12)	-0.0102 (12)
C25	0.0625 (17)	0.0245 (14)	0.0270 (13)	-0.0068 (13)	-0.0123 (13)	0.0007 (12)
C26	0.0503 (15)	0.0342 (15)	0.0194 (12)	-0.0115 (13)	0.0036 (11)	-0.0036 (12)
C27	0.0312 (12)	0.0263 (13)	0.0231 (12)	-0.0055 (11)	-0.0005 (10)	-0.0060 (11)
O28	0.0319 (8)	0.0434 (11)	0.0290 (9)	0.0008 (8)	0.0089 (7)	-0.0014 (8)
C29	0.0358 (14)	0.066 (2)	0.0321 (14)	-0.0049 (14)	0.0089 (12)	-0.0082 (14)

Geometric parameters (Å, °)

Cd1—N2	2.2724 (19)	C16—H16	0.9500
Cd1—N1	2.3142 (18)	C17—O18	1.367 (3)
Cd1—N11	2.3653 (17)	O18—C19	1.429 (3)
Cd1—N21	2.3718 (17)	C19—H19A	0.9800
Cd1—S1 ⁱ	2.7306 (6)	C19—H19B	0.9800

Cd1—S2 ⁱⁱ	2.7449 (6)	C19—H19C	0.9800
S1—C1	1.649 (2)	N21—C22	1.431 (3)
S1—Cd1 ⁱ	2.7306 (6)	N21—H21A	0.9200
C1—N1	1.154 (3)	N21—H21B	0.9200
S2—C2	1.653 (2)	C22—C23	1.376 (3)
S2—Cd1 ⁱⁱⁱ	2.7449 (5)	C22—C27	1.403 (3)
N2—C2	1.152 (3)	C23—C24	1.394 (3)
N11—C12	1.430 (3)	C23—H23	0.9500
N11—H11A	0.9200	C24—C25	1.379 (3)
N11—H11B	0.9200	C24—H24	0.9500
C12—C13	1.377 (3)	C25—C26	1.395 (3)
C12—C17	1.399 (3)	C25—H25	0.9500
C13—C14	1.394 (3)	C26—C27	1.383 (3)
C13—H13	0.9500	C26—H26	0.9500
C14—C15	1.375 (4)	C27—O28	1.365 (3)
C14—H14	0.9500	O28—C29	1.427 (3)
C15—C16	1.389 (4)	C29—H29A	0.9800
C15—H15	0.9500	C29—H29B	0.9800
C16—C17	1.385 (3)	C29—H29C	0.9800
N2—Cd1—N1	175.76 (6)	O18—C17—C16	125.9 (2)
N2—Cd1—N11	88.20 (6)	O18—C17—C12	114.0 (2)
N1—Cd1—N11	92.22 (6)	C16—C17—C12	120.0 (2)
N2—Cd1—N21	95.50 (7)	C17—O18—C19	117.6 (2)
N1—Cd1—N21	84.29 (6)	O18—C19—H19A	109.5
N11—Cd1—N21	175.44 (6)	O18—C19—H19B	109.5
N2—Cd1—S1 ⁱ	91.92 (5)	H19A—C19—H19B	109.5
N1—Cd1—S1 ⁱ	92.31 (4)	O18—C19—H19C	109.5
N11—Cd1—S1 ⁱ	87.74 (4)	H19A—C19—H19C	109.5
N21—Cd1—S1 ⁱ	89.47 (5)	H19B—C19—H19C	109.5
N2—Cd1—S2 ⁱⁱ	93.16 (5)	C22—N21—Cd1	120.21 (13)
N1—Cd1—S2 ⁱⁱ	82.60 (4)	C22—N21—H21A	107.3
N11—Cd1—S2 ⁱⁱ	92.54 (4)	Cd1—N21—H21A	107.3
N21—Cd1—S2 ⁱⁱ	89.92 (5)	C22—N21—H21B	107.3
S1 ⁱ —Cd1—S2 ⁱⁱ	174.914 (18)	Cd1—N21—H21B	107.3
C1—S1—Cd1 ⁱ	99.97 (7)	H21A—N21—H21B	106.9
N1—C1—S1	178.8 (2)	C23—C22—C27	119.8 (2)
C1—N1—Cd1	158.10 (18)	C23—C22—N21	122.1 (2)
C2—S2—Cd1 ⁱⁱⁱ	109.52 (7)	C27—C22—N21	118.0 (2)
C2—N2—Cd1	164.95 (17)	C22—C23—C24	120.3 (2)
N2—C2—S2	178.0 (2)	C22—C23—H23	119.9
C12—N11—Cd1	116.38 (13)	C24—C23—H23	119.9
C12—N11—H11A	108.2	C25—C24—C23	119.9 (2)
Cd1—N11—H11A	108.2	C25—C24—H24	120.0
C12—N11—H11B	108.2	C23—C24—H24	120.0
Cd1—N11—H11B	108.2	C24—C25—C26	120.4 (2)
H11A—N11—H11B	107.3	C24—C25—H25	119.8
C13—C12—C17	119.8 (2)	C26—C25—H25	119.8

C13—C12—N11	121.6 (2)	C27—C26—C25	119.7 (2)
C17—C12—N11	118.52 (19)	C27—C26—H26	120.2
C12—C13—C14	120.1 (2)	C25—C26—H26	120.2
C12—C13—H13	119.9	O28—C27—C26	125.7 (2)
C14—C13—H13	119.9	O28—C27—C22	114.4 (2)
C15—C14—C13	119.8 (2)	C26—C27—C22	120.0 (2)
C15—C14—H14	120.1	C27—O28—C29	117.82 (19)
C13—C14—H14	120.1	O28—C29—H29A	109.5
C14—C15—C16	120.7 (2)	O28—C29—H29B	109.5
C14—C15—H15	119.6	H29A—C29—H29B	109.5
C16—C15—H15	119.6	O28—C29—H29C	109.5
C17—C16—C15	119.4 (2)	H29A—C29—H29C	109.5
C17—C16—H16	120.3	H29B—C29—H29C	109.5
C15—C16—H16	120.3		
N11—Cd1—N1—C1	-141.7 (4)	C13—C12—C17—C16	-1.7 (3)
N21—Cd1—N1—C1	35.3 (4)	N11—C12—C17—C16	175.03 (19)
S1 ⁱ —Cd1—N1—C1	-53.9 (4)	C16—C17—O18—C19	-4.3 (3)
S2 ⁱⁱ —Cd1—N1—C1	126.0 (4)	C12—C17—O18—C19	176.0 (2)
N11—Cd1—N2—C2	-122.1 (7)	N2—Cd1—N21—C22	-16.79 (16)
N21—Cd1—N2—C2	60.6 (7)	N1—Cd1—N21—C22	158.96 (16)
S1 ⁱ —Cd1—N2—C2	150.2 (7)	S1 ⁱ —Cd1—N21—C22	-108.66 (15)
S2 ⁱⁱ —Cd1—N2—C2	-29.6 (7)	S2 ⁱⁱ —Cd1—N21—C22	76.39 (15)
N2—Cd1—N11—C12	-171.56 (15)	Cd1—N21—C22—C23	-90.3 (2)
N1—Cd1—N11—C12	12.66 (14)	Cd1—N21—C22—C27	87.6 (2)
S1 ⁱ —Cd1—N11—C12	-79.56 (14)	C27—C22—C23—C24	0.0 (3)
S2 ⁱⁱ —Cd1—N11—C12	95.35 (14)	N21—C22—C23—C24	177.95 (19)
Cd1—N11—C12—C13	91.3 (2)	C22—C23—C24—C25	-0.5 (3)
Cd1—N11—C12—C17	-85.4 (2)	C23—C24—C25—C26	0.4 (4)
C17—C12—C13—C14	0.2 (3)	C24—C25—C26—C27	0.3 (4)
N11—C12—C13—C14	-176.4 (2)	C25—C26—C27—O28	179.3 (2)
C12—C13—C14—C15	1.3 (4)	C25—C26—C27—C22	-0.8 (3)
C13—C14—C15—C16	-1.2 (4)	C23—C22—C27—O28	-179.42 (19)
C14—C15—C16—C17	-0.3 (4)	N21—C22—C27—O28	2.6 (3)
C15—C16—C17—O18	-178.0 (2)	C23—C22—C27—C26	0.6 (3)
C15—C16—C17—C12	1.7 (3)	N21—C22—C27—C26	-177.39 (19)
C13—C12—C17—O18	178.09 (19)	C26—C27—O28—C29	-8.1 (3)
N11—C12—C17—O18	-5.2 (3)	C22—C27—O28—C29	172.00 (19)

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

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N11—H11A...S2 ⁱⁱⁱ	0.92	2.50	3.4182 (17)	174
N21—H21B...S1 ^{iv}	0.92	2.66	3.5637 (18)	169

N11—H11B···O18	0.92	2.28	2.641 (2)	103
N21—H21A···O28	0.92	2.26	2.640 (2)	104

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