

Poly[tris[μ_2 -2-(pyrazol-1-yl)pyrazine]-hexa- $\mu_{1,3}$ -thiocyanato-tricadmium(II)]

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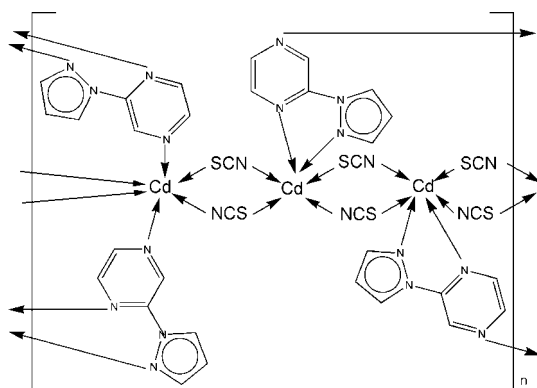
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.022; wR factor = 0.056; data-to-parameter ratio = 14.3.

The asymmetric unit of the title crystal structure, $[\text{Cd}_3(\text{NCS})_6(\text{C}_7\text{H}_6\text{N}_4)_2]_n$, contains two independent Cd^{II} ions, one of which is located on a crystallographic inversion center. Each independent Cd^{II} ion is in a slightly distorted octahedral coordination environment, but the distortion from ideally octahedral is greater in the environment of the Cd^{II} ion on a general position. Both thiocyanate ligands act as bridges connecting independent Cd^{II} ions, and the 2-(pyrazol-1-yl)pyrazine ligands chelate one Cd^{II} ion in a bidentate mode while the remaining N atom of the pyrazine ring coordinates to a symmetry-related Cd^{II} ion, forming a two-dimensional structure parallel to (211).

Related literature

For background information, see: Shi, Sun, Liu *et al.* (2006); Shi, Sun, Zhang *et al.* (2006).



Experimental

Crystal data

$[\text{Cd}_3(\text{NCS})_6(\text{C}_7\text{H}_6\text{N}_4)_2]$
 $M_r = 978.00$
 Triclinic, $P\bar{1}$
 $a = 7.0309$ (9) Å
 $b = 8.6178$ (12) Å
 $c = 13.7373$ (18) Å
 $\alpha = 87.889$ (2)°
 $\beta = 85.173$ (2)°

$\gamma = 68.060$ (2)°
 $V = 769.32$ (18) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 2.50$ mm⁻¹
 $T = 298$ (2) K
 $0.38 \times 0.16 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.450$, $T_{\text{max}} = 0.788$

4043 measured reflections
 2805 independent reflections
 2625 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
 $wR(F^2) = 0.056$
 $S = 1.06$
 2805 reflections

196 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.61$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.51$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—N2	2.286 (3)	Cd2—N5	2.385 (2)
Cd1—N7 ⁱ	2.426 (2)	Cd2—N4	2.436 (2)
Cd1—S2	2.6832 (8)	Cd2—S1	2.6603 (9)
Cd2—N1 ⁱⁱ	2.244 (2)	Cd2—S3	2.7427 (8)
Cd2—N3	2.303 (3)		

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2704).

References

- Bruker (1997). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Shi, J.-M., Sun, Y.-M., Liu, Z., Liu, L.-D., Shi, W. & Cheng, P. (2006). *Dalton Trans.* pp. 376–380.
 Shi, J.-M., Sun, Y.-M., Zhang, X., Yi, L., Cheng, P. & Liu, L.-D. (2006). *J. Phys. Chem. A*, **110**, 7677–7681.

supplementary materials

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Poly[tris[μ_2 -2-(pyrazol-1-yl)pyrazine]hexa- $\mu_{1,3}$ -thiocyanato-tricadmium(II)]

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Comment

For a considerable time, interest has focused on polymeric coordination compounds because such new coordination polymers may afford new materials with useful properties, such as catalytic activity, micro-porosity, electrical conductivity, non-linear optical activity and magnetic coupling behavior. The thiocyanide anion is a very common bridging ligand and many multi-nuclear complexes containing this ligand have been reported. Some of these complexes exhibit interesting magnetic coupling properties (Shi, Sun, Liu *et al.*, 2006; Shi, Sun, Zhang *et al.*, 2006). The 2-(pyrazole-1-yl)-pyrazine molecule can act as a bridge ligand due to its structural character and up till now no crystal structures of complexes with this ligand have been reported. Under the motivation of preparing new coordination polymers containing mixed bridging ligands, we have synthesized the title coordination polymer and herein we report its crystal structure (I).

Fig. 1 shows the coordination around each independent Cd^{II} ion. Atom Cd1 is located on a crystallographic inversion center. In the crystal structure thiocyanate anions act as bridging ligands and connect symmetry related Cd^{II} ions [with Cd...Cd = 5.8122 (6) Å for Cd1...Cd2 and 5.7411 (7) Å for Cd2...Cd2ⁱⁱ; symmetry code: (ii) -x+1, -y+1, -z+1] forming an eight-membered ring which acts as a repeat unit of the structure in one-dimension [Fig. 2]. The 2-(pyrazole-1-yl)-pyrazine ligand functions as a tridentate bridging ligand and coordinates to symmetry related Cd^{II} ions [with a Cd...Cd separation of 7.6144 (7) Å] connecting the structure further into two-dimensions. Figure 2 also shows that in the two-dimensional structure there are two different types of rings formed by the 2-(pyrazole-1-yl)-pyrazine bridging ligand. An 18-membered ring consists of four Cd^{II} ions, two thiocyanato ligands and two 2-(pyrazole-1-yl)-pyrazine bridging ligands while a 26-membered ring consists of two 2-(pyrazole-1-yl)-pyrazine bridging ligands, four thiocyanate ligands and six Cd^{II} ions. The 18-membered rings and the 26-membered rings are arranged alternately in the two-dimensional structure.

Experimental

7 ml 3-(pyrazole-2-yloxy)-pyridine (0.0365 g, 0.250 mmol) methanol solution, 7 ml Cd(ClO₄)₂·6H₂O (0.1048 g, 0.250 mmol) H₂O solution and 4 ml NaSCN (0.0405 g, 0.500 mmol) H₂O solution were mixed together and stirred for a few minutes. Colorless single crystals were obtained after allowing the filtrate to stand at room temperature for four months.

Refinement

All H atoms were placed in calculated positions and refined as riding with (C—H = 0.93 Å) and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$.

Figures

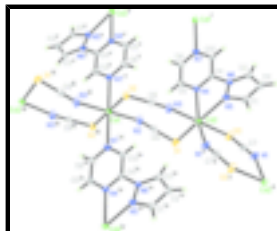


Fig. 1. Coordination around the two independent Cd^{II} ions in (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry codes: (i) $x-1, y+1, z$ (ii) $-x+1, -y+1, -z+1$ (iii) $-x+1, -y, -z$ (iv) $x+1, y-1, z$ (v) $-x, -y+1, -z$].

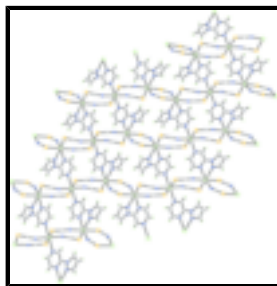


Fig. 2. Part of the two-dimensional sheet structure of (I).

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Crystal data

[Cd₃(NCS)₆(C₇H₆N₄)₂]

$M_r = 978.00$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.0309$ (9) Å

$b = 8.6178$ (12) Å

$c = 13.7373$ (18) Å

$\alpha = 87.889$ (2)°

$\beta = 85.173$ (2)°

$\gamma = 68.060$ (2)°

$V = 769.32$ (18) Å³

$Z = 1$

$F_{000} = 470$

$D_x = 2.111$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3404 reflections

$\theta = 2.6$ – 28.2 °

$\mu = 2.50$ mm⁻¹

$T = 298$ (2) K

Bar, colorless

$0.38 \times 0.16 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.450$, $T_{\max} = 0.788$

4043 measured reflections

2805 independent reflections

2625 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.013$

$\theta_{\text{max}} = 25.5$ °

$\theta_{\text{min}} = 2.6$ °

$h = -4 \rightarrow 8$

$k = -10 \rightarrow 10$

$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0271P)^2 + 0.3586P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
2805 reflections	$(\Delta/\sigma)_{\max} = 0.001$
196 parameters	$\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0009 (4)	0.7101 (4)	0.49099 (19)	0.0358 (6)
H1	0.0564	0.6478	0.5456	0.043*
C2	-0.1423 (5)	0.8730 (4)	0.4948 (2)	0.0402 (7)
H2	-0.1990	0.9378	0.5502	0.048*
C3	-0.1821 (5)	0.9178 (4)	0.4006 (2)	0.0383 (7)
H3	-0.2725	1.0200	0.3788	0.046*
C4	-0.0578 (4)	0.7640 (3)	0.24350 (18)	0.0260 (5)
C5	0.1109 (5)	0.6225 (4)	0.1068 (2)	0.0381 (7)
H5	0.2239	0.5397	0.0758	0.046*
C6	-0.0462 (5)	0.7197 (4)	0.0532 (2)	0.0388 (7)
H6	-0.0368	0.7019	-0.0137	0.047*
C7	0.5004 (4)	0.6931 (3)	0.4694 (2)	0.0312 (6)
C8	0.2476 (4)	0.1598 (3)	0.21816 (19)	0.0309 (6)
C9	0.6045 (4)	0.3004 (4)	0.1046 (2)	0.0369 (7)
C13	-0.2187 (4)	0.8625 (3)	0.18960 (19)	0.0311 (6)
H13	-0.3319	0.9454	0.2206	0.037*
Cd1	0.5000	0.0000	0.0000	0.02922 (9)
Cd2	0.35673 (3)	0.47371 (2)	0.314014 (13)	0.02935 (8)

supplementary materials

N1	0.5156 (4)	0.6693 (3)	0.55123 (18)	0.0419 (6)
N2	0.5526 (4)	0.2304 (3)	0.04926 (19)	0.0445 (6)
N3	0.2614 (4)	0.2620 (3)	0.26533 (18)	0.0438 (6)
N4	0.1055 (3)	0.6441 (3)	0.20341 (16)	0.0298 (5)
N5	0.0489 (3)	0.6539 (3)	0.40006 (16)	0.0311 (5)
N6	-0.0646 (3)	0.7848 (3)	0.34443 (15)	0.0292 (5)
N7	-0.2124 (3)	0.8392 (3)	0.09389 (16)	0.0325 (5)
S1	0.67535 (14)	0.40534 (14)	0.18169 (7)	0.0617 (3)
S2	0.22912 (12)	0.01127 (9)	0.15191 (5)	0.03591 (17)
S3	0.47355 (13)	0.73397 (10)	0.35252 (5)	0.04143 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0406 (16)	0.0454 (16)	0.0255 (14)	-0.0200 (14)	-0.0055 (12)	0.0002 (12)
C2	0.0428 (17)	0.0477 (17)	0.0322 (15)	-0.0193 (14)	0.0024 (13)	-0.0120 (13)
C3	0.0397 (16)	0.0325 (15)	0.0388 (16)	-0.0084 (13)	-0.0025 (13)	-0.0082 (12)
C4	0.0233 (13)	0.0304 (13)	0.0244 (13)	-0.0100 (11)	-0.0017 (10)	0.0002 (10)
C5	0.0332 (15)	0.0398 (16)	0.0282 (14)	0.0017 (13)	-0.0024 (12)	-0.0046 (12)
C6	0.0380 (16)	0.0445 (16)	0.0243 (14)	-0.0040 (13)	-0.0039 (12)	-0.0001 (12)
C7	0.0316 (14)	0.0281 (13)	0.0344 (16)	-0.0105 (11)	-0.0082 (12)	-0.0009 (11)
C8	0.0312 (15)	0.0360 (15)	0.0247 (13)	-0.0121 (12)	-0.0023 (11)	0.0042 (12)
C9	0.0312 (15)	0.0371 (15)	0.0368 (16)	-0.0075 (13)	0.0061 (12)	-0.0059 (13)
C13	0.0250 (13)	0.0337 (14)	0.0285 (14)	-0.0036 (11)	-0.0035 (11)	0.0007 (11)
Cd1	0.02909 (16)	0.03095 (15)	0.02367 (15)	-0.00539 (12)	-0.00732 (11)	-0.00178 (11)
Cd2	0.02855 (12)	0.03169 (12)	0.02402 (12)	-0.00559 (9)	-0.00708 (8)	-0.00237 (8)
N1	0.0545 (16)	0.0386 (14)	0.0348 (14)	-0.0171 (12)	-0.0183 (12)	0.0057 (11)
N2	0.0539 (17)	0.0435 (15)	0.0377 (14)	-0.0203 (13)	0.0023 (12)	-0.0115 (12)
N3	0.0551 (17)	0.0472 (15)	0.0326 (13)	-0.0228 (13)	-0.0010 (12)	-0.0081 (12)
N4	0.0251 (11)	0.0327 (12)	0.0280 (12)	-0.0062 (10)	-0.0057 (9)	0.0008 (9)
N5	0.0288 (12)	0.0353 (12)	0.0266 (11)	-0.0088 (10)	-0.0045 (9)	0.0028 (9)
N6	0.0260 (11)	0.0327 (12)	0.0263 (11)	-0.0072 (9)	-0.0057 (9)	-0.0008 (9)
N7	0.0271 (12)	0.0367 (12)	0.0283 (12)	-0.0053 (10)	-0.0056 (10)	0.0032 (10)
S1	0.0419 (5)	0.0957 (7)	0.0566 (5)	-0.0359 (5)	0.0139 (4)	-0.0407 (5)
S2	0.0423 (4)	0.0402 (4)	0.0301 (4)	-0.0209 (3)	-0.0007 (3)	-0.0051 (3)
S3	0.0571 (5)	0.0523 (5)	0.0274 (4)	-0.0342 (4)	-0.0067 (3)	0.0023 (3)

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

C1—N5	1.327 (3)	C9—N2	1.148 (4)
C1—C2	1.388 (4)	C9—S1	1.639 (3)
C1—H1	0.9300	C13—N7	1.332 (3)
C2—C3	1.359 (4)	C13—H13	0.9300
C2—H2	0.9300	Cd1—N2	2.286 (3)
C3—N6	1.357 (3)	Cd1—N2 ⁱ	2.286 (3)
C3—H3	0.9300	Cd1—N7 ⁱⁱ	2.426 (2)
C4—N4	1.319 (3)	Cd1—N7 ⁱⁱⁱ	2.426 (2)
C4—C13	1.388 (4)	Cd1—S2 ⁱ	2.6832 (8)

C4—N6	1.399 (3)	Cd1—S2	2.6832 (8)
C5—N4	1.342 (3)	Cd2—N1 ^{iv}	2.244 (2)
C5—C6	1.365 (4)	Cd2—N3	2.303 (3)
C5—H5	0.9300	Cd2—N5	2.385 (2)
C6—N7	1.331 (4)	Cd2—N4	2.436 (2)
C6—H6	0.9300	Cd2—S1	2.6603 (9)
C7—N1	1.142 (3)	Cd2—S3	2.7427 (8)
C7—S3	1.643 (3)	N1—Cd2 ^{iv}	2.244 (2)
C8—N3	1.150 (4)	N5—N6	1.364 (3)
C8—S2	1.647 (3)	N7—Cd1 ^v	2.426 (2)
N5—C1—C2	111.8 (3)	N7 ⁱⁱ —Cd1—S2	91.66 (6)
N5—C1—H1	124.1	N7 ⁱⁱⁱ —Cd1—S2	88.34 (6)
C2—C1—H1	124.1	S2 ⁱ —Cd1—S2	180
C3—C2—C1	105.6 (3)	N1 ^{iv} —Cd2—N3	91.59 (9)
C3—C2—H2	127.2	N1 ^{iv} —Cd2—N5	93.71 (9)
C1—C2—H2	127.2	N3—Cd2—N5	102.07 (9)
N6—C3—C2	106.9 (3)	N1 ^{iv} —Cd2—N4	159.57 (9)
N6—C3—H3	126.6	N3—Cd2—N4	83.77 (9)
C2—C3—H3	126.6	N5—Cd2—N4	68.04 (7)
N4—C4—C13	122.2 (2)	N1 ^{iv} —Cd2—S1	105.57 (8)
N4—C4—N6	116.7 (2)	N3—Cd2—S1	94.46 (7)
C13—C4—N6	121.1 (2)	N5—Cd2—S1	154.21 (6)
N4—C5—C6	121.4 (3)	N4—Cd2—S1	94.63 (6)
N4—C5—H5	119.3	N1 ^{iv} —Cd2—S3	93.51 (7)
C6—C5—H5	119.3	N3—Cd2—S3	174.25 (7)
N7—C6—C5	121.9 (3)	N5—Cd2—S3	80.27 (6)
N7—C6—H6	119.0	N4—Cd2—S3	92.33 (6)
C5—C6—H6	119.0	S1—Cd2—S3	81.60 (3)
N1—C7—S3	178.1 (3)	C7—N1—Cd2 ^{iv}	156.4 (2)
N3—C8—S2	179.1 (3)	C9—N2—Cd1	151.9 (3)
N2—C9—S1	178.3 (3)	C8—N3—Cd2	160.7 (2)
N7—C13—C4	120.5 (2)	C4—N4—C5	116.7 (2)
N7—C13—H13	119.7	C4—N4—Cd2	116.51 (17)
C4—C13—H13	119.7	C5—N4—Cd2	126.65 (18)
N2—Cd1—N2 ⁱ	180	C1—N5—N6	104.4 (2)
N2—Cd1—N7 ⁱⁱ	85.94 (9)	C1—N5—Cd2	134.13 (19)
N2 ⁱ —Cd1—N7 ⁱⁱ	94.06 (9)	N6—N5—Cd2	112.89 (15)
N2—Cd1—N7 ⁱⁱⁱ	94.06 (9)	C3—N6—N5	111.4 (2)
N2 ⁱ —Cd1—N7 ⁱⁱⁱ	85.94 (9)	C3—N6—C4	129.3 (2)
N7 ⁱⁱ —Cd1—N7 ⁱⁱⁱ	180	N5—N6—C4	119.2 (2)
N2—Cd1—S2 ⁱ	86.38 (7)	C6—N7—C13	117.2 (2)
N2 ⁱ —Cd1—S2 ⁱ	93.62 (7)	C6—N7—Cd1 ^v	121.71 (18)
N7 ⁱⁱ —Cd1—S2 ⁱ	88.34 (6)	C13—N7—Cd1 ^v	120.98 (18)
N7 ⁱⁱⁱ —Cd1—S2 ⁱ	91.66 (6)	C9—S1—Cd2	98.65 (11)

supplementary materials

N2—Cd1—S2	93.62 (7)	C8—S2—Cd1	101.07 (10)
N2 ⁱ —Cd1—S2	86.38 (7)	C7—S3—Cd2	96.52 (10)
N5—C1—C2—C3	-0.3 (4)	S1—Cd2—N5—C1	-110.8 (3)
C1—C2—C3—N6	-0.3 (3)	S3—Cd2—N5—C1	-64.9 (3)
N4—C5—C6—N7	-0.5 (5)	N1 ^{iv} —Cd2—N5—N6	169.76 (17)
N4—C4—C13—N7	-0.5 (4)	N3—Cd2—N5—N6	-97.82 (18)
N6—C4—C13—N7	-178.6 (2)	N4—Cd2—N5—N6	-19.70 (16)
N7 ⁱⁱ —Cd1—N2—C9	-30.1 (5)	S1—Cd2—N5—N6	30.9 (3)
N7 ⁱⁱⁱ —Cd1—N2—C9	149.9 (5)	S3—Cd2—N5—N6	76.83 (17)
S2 ⁱ —Cd1—N2—C9	-118.7 (5)	C2—C3—N6—N5	0.7 (3)
S2—Cd1—N2—C9	61.3 (5)	C2—C3—N6—C4	176.0 (3)
N1 ^{iv} —Cd2—N3—C8	-124.3 (8)	C1—N5—N6—C3	-0.9 (3)
N5—Cd2—N3—C8	141.6 (8)	Cd2—N5—N6—C3	-153.58 (19)
N4—Cd2—N3—C8	75.7 (8)	C1—N5—N6—C4	-176.7 (2)
S1—Cd2—N3—C8	-18.5 (8)	Cd2—N5—N6—C4	30.6 (3)
C13—C4—N4—C5	0.9 (4)	N4—C4—N6—C3	162.2 (3)
N6—C4—N4—C5	179.1 (3)	C13—C4—N6—C3	-19.5 (4)
C13—C4—N4—Cd2	-175.6 (2)	N4—C4—N6—N5	-22.8 (3)
N6—C4—N4—Cd2	2.7 (3)	C13—C4—N6—N5	155.5 (2)
C6—C5—N4—C4	-0.4 (4)	C5—C6—N7—C13	1.0 (5)
C6—C5—N4—Cd2	175.7 (2)	C5—C6—N7—Cd1 ^v	-176.2 (2)
N1 ^{iv} —Cd2—N4—C4	37.2 (3)	C4—C13—N7—C6	-0.5 (4)
N3—Cd2—N4—C4	114.9 (2)	C4—C13—N7—Cd1 ^v	176.70 (19)
N5—Cd2—N4—C4	9.15 (18)	N1 ^{iv} —Cd2—S1—C9	113.39 (13)
S1—Cd2—N4—C4	-151.14 (18)	N3—Cd2—S1—C9	20.49 (14)
S3—Cd2—N4—C4	-69.38 (19)	N5—Cd2—S1—C9	-109.59 (17)
N1 ^{iv} —Cd2—N4—C5	-138.9 (3)	N4—Cd2—S1—C9	-63.61 (13)
N3—Cd2—N4—C5	-61.2 (3)	S3—Cd2—S1—C9	-155.29 (12)
N5—Cd2—N4—C5	-166.9 (3)	N2—Cd1—S2—C8	-7.34 (12)
S1—Cd2—N4—C5	32.8 (2)	N2 ⁱ —Cd1—S2—C8	172.66 (12)
S3—Cd2—N4—C5	114.6 (2)	N7 ⁱⁱ —Cd1—S2—C8	78.70 (11)
C2—C1—N5—N6	0.7 (3)	N7 ⁱⁱⁱ —Cd1—S2—C8	-101.30 (11)
C2—C1—N5—Cd2	144.6 (2)	N1 ^{iv} —Cd2—S3—C7	-19.29 (12)
N1 ^{iv} —Cd2—N5—C1	28.0 (3)	N5—Cd2—S3—C7	73.89 (11)
N3—Cd2—N5—C1	120.4 (3)	N4—Cd2—S3—C7	141.13 (11)
N4—Cd2—N5—C1	-161.5 (3)	S1—Cd2—S3—C7	-124.53 (11)

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

Fig. 1

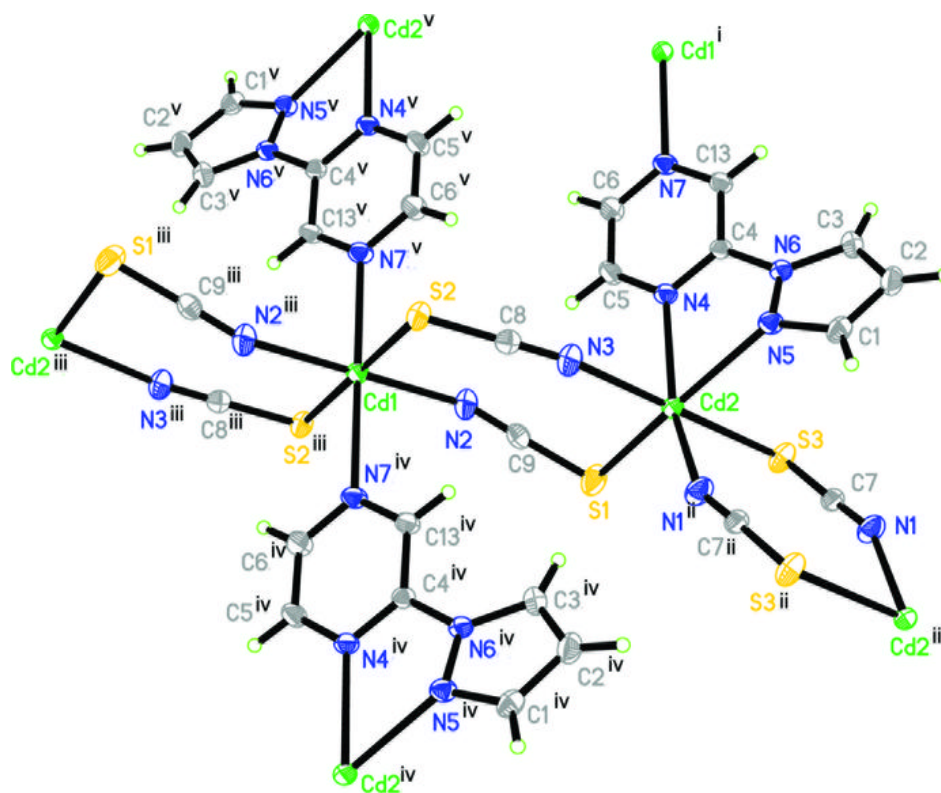


Fig. 2

