Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(2-aminothiazole-κN)-cadmium(II)]-di-μ-thiocyanato-$\kappa^2N:S;\kappa^2S:N$]

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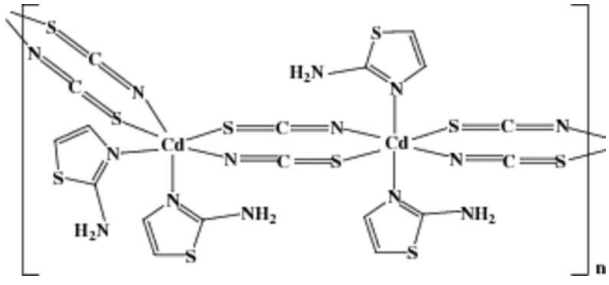
Received 6 July 2007; accepted 11 July 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.028; wR factor = 0.078; data-to-parameter ratio = 17.1.

There are two independent Cd atoms in the title compound, $[Cd(NCS)_2(C_3H_4N_2S)_2]_n$; one lies on a twofold rotation axis and another is situated on an inversion center, but they are each in a distorted octahedral environment within N_4S_2 donor sets. One NH_2 group is disordered equally over two positions. Each Cd atom is doubly bridged by thiocyanate ligands to neighboring Cd atoms. The 2-aminothiazole ligands are alternately coordinated to one Cd atom in a *cis* conformation and to the other Cd atom in a *trans* conformation. Overall, the structure is a one-dimensional zigzag chain.

Related literature

For related literature, see: Balch *et al.* (1993); Braga *et al.* (1998); Costes *et al.* (1991); Kim *et al.* (2004); Raper *et al.* (1984); Suh *et al.* (2005); Vrieze & Koten (1987).



Experimental

Crystal data

$[Cd(NCS)_2(C_3H_4N_2S)_2]$
M_r = 428.84
Monoclinic, $C2/c$
a = 18.7079 (18) Å
b = 9.0553 (13) Å
c = 18.661 (2) Å
β = 110.918 (8)°
V = 2953.0 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.04 mm^{-1}
T = 295 (2) K
0.43 × 0.31 × 0.28 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: φ scan (*XSCANS*; Bruker, 1996)
T_{min} = 0.474, T_{max} = 0.599
(expected range = 0.447–0.565)
3784 measured reflections
3046 independent reflections
2860 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.078
S = 1.11
3046 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—S1	2.7422 (11)	Cd2—S4	2.7616 (9)
Cd1—N6	2.336 (3)	Cd2—N3	2.302 (3)
Cd1—N13	2.328 (3)	Cd2—N23	2.373 (3)
S1^{i}—Cd1—S1	90.85 (7)	N3^{ii}—Cd2—N3	180
N6—Cd1—S1	96.40 (7)	N3—Cd2—S4	94.17 (8)
N6—Cd1—N6^{i}	178.08 (14)	N3—Cd2—N23	90.27 (10)
N13—Cd1—S1	91.73 (8)	S4—Cd2—S4^{ii}	180
N13—Cd1—S1^{i}	169.74 (7)	N23—Cd2—S4	90.82 (7)
N13—Cd1—N6	87.61 (10)	N23—Cd2—N23^{ii}	180
N13—Cd1—N13^{i}	87.47 (15)		

Symmetry codes: (i) $-x, y, -z+\frac{1}{2}$; (ii) $-x-\frac{1}{2}, -y+\frac{3}{2}, -z$.

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); 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: TK2178).

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 doi:10.1107/S1600536807033983

supplementary materials

Acta Cryst. (2007). E**63**, m2177 [**doi:10.1107/S1600536807033983**]

catena-Poly[[bis(2-aminothiazole-κN)cadmium(II)]-di-μ-thiocyanato-$\kappa^2 N$:S;$\kappa^2 S$:N]

S. W. Suh, C.-H. Kim and I. H. Kim

Comment

Crystal engineering of coordination complexes is motivated by the development of materials with useful properties such as catalytic, magnetic, electronic and optical (Braga *et al.*, 1998). The pseudo-halide ions, *e.g.* CN^-, SCN^-, N_3^-, are known to build up 1-, 2- and 3-D structures by bridging metal centers (Vrieze & Koten, 1987). Using complementary organic ligands, such as aliphatic and aromatic amines, is known to play an important role in stabilizing multi-dimensional structures. Especially, aromatic heterocycles such as imidazole and thiazole derivatives represent an important class of ligands in coordination chemistry. A number of metal complexes of various imidazole derivatives have been synthesized and characterized (Balch *et al.*, 1993; Costes *et al.*, 1991). However, the frameworks of metal complexes containing thiazole derivatives have been considerably less investigated. Our research is focused on the development of novel supramolecular framework structures (Kim *et al.*, 2004; Suh *et al.*, 2005) utilizing the terminal and bridging properties of pseudo-halide ions, and the coordination behaviour of imidazole or thiazole derivatives as complementary organic ligands. Herein, we present the synthesis and structure determination of a cadmium(II) thiocyanato complex, (I), with 2-aminothiazole, Fig. 1. Each Cd atom has an octahedral geometry being hexa-coordinated by two amino-N atoms of 2-aminothiazole, and two N and two S atoms derived from four thiocyanate ligands. The 2-aminothiazole ligands are coordinated to the Cd(1) atom, which lies on a center of inversion, in a *cis*-conformation and to the Cd(2) atom, which lies on a 2-fold axis, in a *trans* manner. With the aforementioned bridging, an infinite 1-D zigzag chain results. Bond lengths and angles, Table 1, of the 2-aminothiazole ligand are similar to the related compound, tetrakis(2-aminothiazole)bis(isothiocyanate)cobalt(II) (Raper *et al.*, 1984).

Experimental

A water-methanolic (2:1) solution (30 ml) of potassium thiocyanate (9 mmol, 0.88 g) was added to a water-methanolic (2:1) solution (30 ml) of $Cd(NO_3)\cdot 4H_2O$ (3 mmol, 0.93 g). To this mixture solution, a water-methanolic (2:1) solution (30 ml) of 2-aminothiazole (10 mmol, 1.00 g) was introduced, with stirring. The small amount of precipitates formed from the resulting solution were filtered off. The filtered solution was allowed to stand at room temperature. After a few days dark-yellow block crystals suitable for X-ray analysis were obtained. Analysis found: C 22.45, H 1.82, Cd 26.20, N 19.63, S 30.48%; $C_8H_8CdN_6S_4$ requires: C 22.40, H 1.88, Cd 26.21, N 19.60, S 29.90%.

Refinement

The 2-aminothiazole-N16 atom was found to be disordered over two positions and from refinement, the final occupancy factors were 0.50. Positional parameters for the H atoms were calculated geometrically and constrained to ride on their attached atoms with C—H = 0.93 Å and N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C, N)$.

Figures

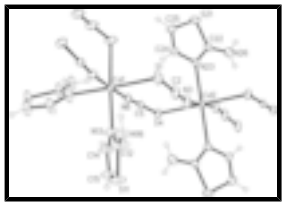

Fig. 1. Portion of the 1-D polymer in (I) showing the coordination geometries for the Cd(II) atoms and the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. The disordered N17 atom of one 2-aminothiazole is omitted for clarity.

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Crystal data

$[Cd(NCS)_2(C_3H_4N_2S)_2]$	F_{000} = 1680
M_r = 428.84	D_x = 1.929 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 42 reflections
a = 18.7079 (18) Å	θ = 4.7–12.5º
b = 9.0553 (13) Å	μ = 2.04 mm^{-1}
c = 18.661 (2) Å	*T* = 295 (2) K
β = 110.918 (8)º	Block, dark-yellow
V = 2953.0 (6) Å^3	0.43 × 0.31 × 0.28 mm
Z = 8	

Data collection

Bruker P4 diffractometer	R_{int} = 0.025
Radiation source: fine-focus sealed tube	θ_{max} = 26.5º
Monochromator: graphite	θ_{min} = 2.3º
T = 295(2) K	*h* = −1→23
2θ/ω scans	*k* = −11→1
Absorption correction: empirical (using intensity measurements) (XSCANS; Bruker, 1996)	*l* = −23→22
T_{min} = 0.474, T_{max} = 0.599	3 standard reflections
3784 measured reflections	every 97 reflections
3046 independent reflections	intensity decay: none
2860 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.028	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 7.3517P]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.11$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
3046 reflections	$\Delta\rho_{min} = -0.76$ e Å^{-3}
178 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00205 (11)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.0000	0.49223 (3)	0.2500	0.03120 (11)	
Cd2	−0.2500	0.7500	0.0000	0.03061 (11)	
S1	0.02580 (6)	0.70476 (14)	0.15739 (7)	0.0705 (4)	
C2	−0.05999 (18)	0.7030 (3)	0.09211 (18)	0.0362 (6)	
N3	−0.12043 (15)	0.7042 (4)	0.04573 (16)	0.0436 (6)	
S4	−0.28158 (4)	0.53426 (11)	0.08902 (5)	0.0418 (2)	
C5	−0.19410 (17)	0.5119 (3)	0.15148 (17)	0.0312 (6)	
N6	−0.13341 (15)	0.4965 (3)	0.19488 (17)	0.0410 (6)	
S11	0.01787 (7)	0.13108 (14)	0.06482 (7)	0.0750 (4)	
C12	0.0430 (3)	0.2810 (5)	0.1256 (3)	0.0649 (13)	
N13	−0.00175 (16)	0.3065 (3)	0.16315 (16)	0.0413 (6)	
C14	−0.0586 (2)	0.2022 (4)	0.1446 (2)	0.0486 (8)	
H14A	−0.0958	0.2019	0.1669	0.058*	
C15	−0.0577 (2)	0.1020 (4)	0.0934 (2)	0.0541 (9)	
H15	−0.0933	0.0264	0.0756	0.065*	
N16	0.1189 (7)	0.3314 (14)	0.1494 (7)	0.079 (4)	0.50
H16A	0.1377	0.3820	0.1909	0.095*	0.50
H16B	0.1466	0.3116	0.1224	0.095*	0.50
N17	0.0918 (7)	0.3884 (15)	0.1145 (6)	0.079 (4)	0.50
H17A	0.0927	0.4756	0.1330	0.095*	0.50
H17B	0.1208	0.3671	0.0891	0.095*	0.50
S21	−0.24556 (6)	1.13954 (10)	0.18452 (6)	0.0539 (2)	
C22	−0.2680 (2)	1.0552 (4)	0.0958 (2)	0.0425 (7)	
N23	−0.23323 (15)	0.9279 (3)	0.09804 (15)	0.0364 (6)	

C24	−0.1856 (2)	0.8968 (4)	0.17249 (18)	0.0441 (7)
H24A	−0.1557	0.8118	0.1847	0.053*
C25	−0.1850 (2)	0.9956 (4)	0.2256 (2)	0.0537 (9)
H25	−0.1559	0.9878	0.2775	0.064*
N26	−0.3175 (2)	1.1158 (4)	0.0324 (2)	0.0675 (10)
H26A	−0.3287	1.0712	−0.0109	0.081*
H26B	−0.3383	1.1995	0.0349	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02668 (17)	0.03422 (18)	0.02801 (17)	0.000	0.00404 (12)	0.000
Cd2	0.02562 (17)	0.03635 (19)	0.02680 (17)	0.00368 (11)	0.00563 (12)	0.00005 (11)
S1	0.0393 (5)	0.0744 (7)	0.0720 (7)	−0.0191 (5)	−0.0118 (5)	0.0359 (6)
C2	0.0349 (16)	0.0333 (15)	0.0392 (16)	0.0035 (12)	0.0117 (13)	0.0099 (13)
N3	0.0300 (14)	0.0555 (17)	0.0416 (15)	0.0058 (12)	0.0085 (12)	0.0088 (13)
S4	0.0267 (4)	0.0563 (5)	0.0364 (4)	−0.0026 (3)	0.0039 (3)	0.0128 (4)
C5	0.0323 (15)	0.0317 (14)	0.0305 (14)	−0.0001 (11)	0.0125 (12)	0.0027 (11)
N6	0.0305 (14)	0.0439 (15)	0.0417 (15)	0.0016 (11)	0.0046 (12)	0.0052 (12)
S11	0.0784 (7)	0.0805 (8)	0.0858 (8)	−0.0401 (6)	0.0535 (7)	−0.0548 (7)
C12	0.068 (3)	0.075 (3)	0.071 (3)	−0.043 (2)	0.047 (2)	−0.045 (2)
N13	0.0401 (14)	0.0470 (16)	0.0429 (14)	−0.0187 (12)	0.0224 (12)	−0.0175 (13)
C14	0.0460 (19)	0.0444 (18)	0.063 (2)	−0.0173 (16)	0.0285 (17)	−0.0110 (17)
C15	0.048 (2)	0.0454 (19)	0.070 (2)	−0.0200 (16)	0.0222 (18)	−0.0173 (18)
N16	0.078 (8)	0.092 (9)	0.095 (8)	−0.052 (6)	0.066 (7)	−0.054 (6)
N17	0.078 (8)	0.092 (9)	0.095 (8)	−0.052 (6)	0.066 (7)	−0.054 (6)
S21	0.0670 (6)	0.0438 (5)	0.0630 (6)	−0.0083 (4)	0.0380 (5)	−0.0182 (4)
C22	0.0494 (19)	0.0349 (16)	0.0509 (19)	−0.0010 (14)	0.0275 (16)	−0.0030 (15)
N23	0.0415 (14)	0.0350 (13)	0.0347 (13)	0.0013 (11)	0.0157 (11)	−0.0018 (11)
C24	0.0522 (19)	0.0434 (18)	0.0362 (16)	−0.0038 (15)	0.0152 (15)	−0.0027 (14)
C25	0.066 (2)	0.057 (2)	0.0404 (19)	−0.0098 (18)	0.0227 (18)	−0.0064 (16)
N26	0.079 (2)	0.0529 (19)	0.062 (2)	0.0277 (18)	0.0156 (19)	0.0011 (17)

Geometric parameters (Å, °)

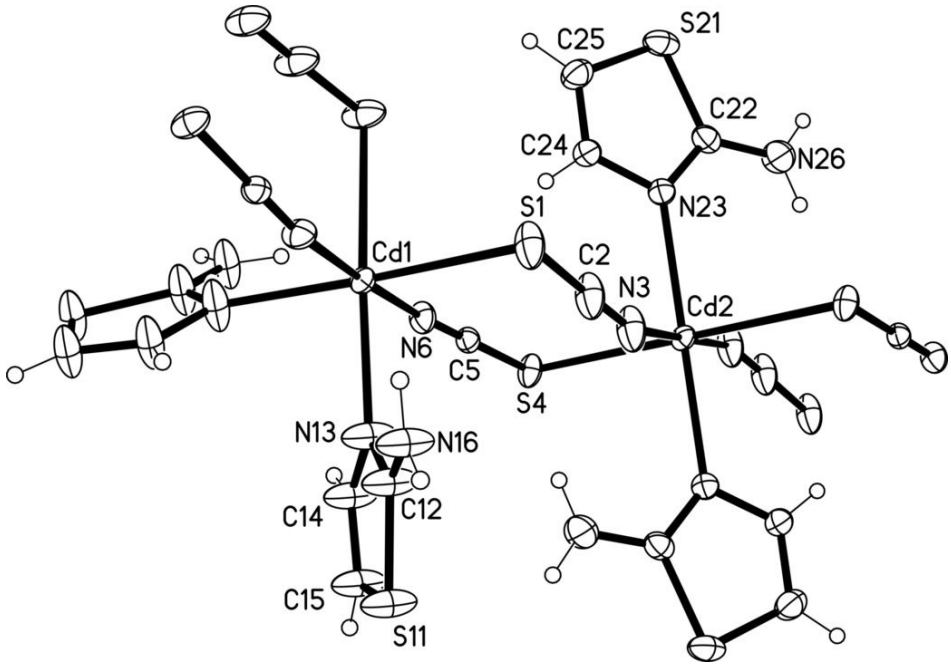
Cd1—S1^{i}	2.7422 (11)	C12—N17	1.399 (13)
Cd1—S1	2.7422 (11)	N13—C14	1.371 (4)
Cd1—N6	2.336 (3)	C14—C15	1.321 (5)
Cd1—N6^{i}	2.336 (3)	C14—H14A	0.9300
Cd1—N13	2.328 (3)	C15—H15	0.9300
Cd1—N13^{i}	2.328 (3)	N16—H16A	0.8600
Cd2—S4	2.7616 (9)	N16—H16B	0.8600
Cd2—N3^{ii}	2.302 (3)	N17—H17A	0.8600
Cd2—N3	2.302 (3)	N17—H17B	0.8600
Cd2—S4^{ii}	2.7616 (9)	S21—C22	1.733 (4)
Cd2—N23	2.373 (3)	S21—C25	1.717 (4)
Cd2—N23^{ii}	2.373 (3)	C22—N23	1.317 (4)

S1—C2	1.632 (3)	C22—N26	1.332 (5)
C2—N3	1.153 (4)	N23—C24	1.386 (4)
S4—C5	1.648 (3)	C24—C25	1.332 (5)
C5—N6	1.144 (4)	C24—H24A	0.9300
S11—C12	1.723 (4)	C25—H25	0.9300
S11—C15	1.701 (4)	N26—H26A	0.8600
C12—N13	1.289 (4)	N26—H26B	0.8600
C12—N16	1.404 (13)		
$S1^{i}$—Cd1—S1	90.85 (7)	C24—N23—Cd2	119.7 (2)
N6—Cd1—S1	96.40 (7)	N3—C2—S1	178.8 (3)
$N6^{i}$—Cd1—S1	82.24 (8)	N6—C5—S4	179.9 (4)
N6—Cd1—$S1^{i}$	82.24 (8)	C12—N13—C14	109.6 (3)
$N6^{i}$—Cd1—$S1^{i}$	96.40 (7)	N13—C12—S11	114.9 (3)
N6—Cd1—$N6^{i}$	178.08 (14)	N13—C12—N16	123.4 (6)
$N13^{i}$—Cd1—$S1^{i}$	91.73 (8)	N13—C12—N17	122.7 (7)
N13—Cd1—S1	91.73 (8)	C14—C15—S11	110.3 (3)
N13—Cd1—$S1^{i}$	169.74 (7)	C15—S11—C12	88.67 (18)
$N13^{i}$—Cd1—S1	169.74 (7)	C15—C14—N13	116.5 (3)
N13—Cd1—N6	87.61 (10)	N16—C12—S11	118.1 (6)
$N13^{i}$—Cd1—N6	93.78 (10)	N17—C12—S11	119.2 (6)
N13—Cd1—$N6^{i}$	93.78 (10)	S11—C15—H15	124.8
$N13^{i}$—Cd1—$N6^{i}$	87.61 (10)	C12—N16—H16A	120.0
N13—Cd1—$N13^{i}$	87.47 (15)	C12—N16—H16B	120.0
$N3^{ii}$—Cd2—N3	180.00 (16)	C12—N17—H17A	120.0
$N3^{ii}$—Cd2—S4	85.83 (8)	C12—N17—H17B	120.0
N3—Cd2—S4	94.17 (8)	N13—C14—H14A	121.7
$N3^{ii}$—Cd2—$S4^{ii}$	94.17 (8)	C14—C15—H15	124.8
N3—Cd2—$S4^{ii}$	85.83 (8)	C15—C14—H14A	121.7
$N3^{ii}$—Cd2—N23	89.73 (10)	H16A—N16—H16B	120.0
N3—Cd2—N23	90.27 (10)	H17A—N17—H17B	120.0
$N3^{ii}$—Cd2—$N23^{ii}$	90.27 (10)	C22—N23—C24	110.1 (3)
N3—Cd2—$N23^{ii}$	89.73 (10)	N23—C22—N26	124.6 (3)
S4—Cd2—$S4^{ii}$	180.00 (3)	N23—C22—S21	114.0 (3)
N23—Cd2—S4	90.82 (7)	C24—C25—S21	110.5 (3)
$N23^{ii}$—Cd2—S4	89.18 (7)	C25—S21—C22	89.30 (17)
N23—Cd2—$S4^{ii}$	89.18 (7)	C25—C24—N23	116.1 (3)
$N23^{ii}$—Cd2—$S4^{ii}$	90.82 (7)	N26—C22—S21	121.4 (3)
N23—Cd2—$N23^{ii}$	180.00 (9)	S21—C25—H25	124.8
C2—S1—Cd1	96.66 (11)	C22—N26—H26A	120.0
C5—N6—Cd1	161.5 (3)	C22—N26—H26B	120.0
C12—N13—Cd1	131.1 (2)	N23—C24—H24A	121.9
C14—N13—Cd1	119.3 (2)	C24—C25—H25	124.8
C2—N3—Cd2	154.3 (3)	C25—C24—H24A	121.9
C5—S4—Cd2	98.09 (10)	H26A—N26—H26B	120.0

C22—N23—Cd2	130.0 (2)		
Cd1—N13—C14—C15	178.2 (3)	N13—Cd1—N6—C5	−65.9 (8)
Cd2—N23—C24—C25	−173.5 (3)	$N13^{i}$—Cd1—N6—C5	−153.2 (8)
$S1^{i}$—Cd1—S1—C2	−97.42 (14)	$N13^{i}$—Cd1—N13—C12	−124.6 (5)
$S1^{i}$—Cd1—N6—C5	115.6 (8)	$N13^{i}$—Cd1—N13—C14	56.3 (3)
S1—Cd1—N6—C5	25.6 (8)	N23—Cd2—N3—C2	22.6 (6)
$S1^{i}$—Cd1—N13—C12	149.7 (4)	$N23^{ii}$—Cd2—N3—C2	−157.4 (6)
S1—Cd1—N13—C12	45.2 (4)	N23—Cd2—S4—C5	−73.06 (13)
$S1^{i}$—Cd1—N13—C14	−29.5 (7)	$N23^{ii}$—Cd2—S4—C5	106.94 (13)
S1—Cd1—N13—C14	−134.0 (3)	S11—C12—N13—Cd1	−178.3 (2)
$N3^{ii}$—Cd2—S4—C5	−162.73 (14)	S11—C12—N13—C14	0.9 (5)
N3—Cd2—S4—C5	17.27 (14)	C12—S11—C15—C14	−0.2 (4)
$N3^{ii}$—Cd2—N23—C22	−37.4 (3)	C12—N13—C14—C15	−1.1 (6)
N3—Cd2—N23—C22	142.6 (3)	N13—C14—C15—S11	0.8 (5)
$N3^{ii}$—Cd2—N23—C24	136.1 (2)	C15—S11—C12—N13	−0.4 (4)
N3—Cd2—N23—C24	−43.9 (2)	C15—S11—C12—N17	−161.1 (7)
S4—Cd2—N3—C2	−68.2 (6)	C15—S11—C12—N16	158.8 (6)
$S4^{ii}$—Cd2—N3—C2	111.8 (6)	N16—C12—N13—Cd1	23.7 (9)
S4—Cd2—N23—C22	−123.2 (3)	N16—C12—N13—C14	−157.1 (7)
$S4^{ii}$—Cd2—N23—C22	56.8 (3)	N17—C12—N13—Cd1	−18.4 (9)
S4—Cd2—N23—C24	50.3 (2)	N17—C12—N13—C14	160.8 (7)
$S4^{ii}$—Cd2—N23—C24	−129.7 (2)	S21—C22—N23—Cd2	172.61 (15)
N6—Cd1—S1—C2	−15.13 (15)	S21—C22—N23—C24	−1.4 (4)
$N6^{i}$—Cd1—S1—C2	166.23 (15)	C22—S21—C25—C24	−0.3 (3)
N6—Cd1—N13—C12	141.5 (4)	C22—N23—C24—C25	1.2 (4)
$N6^{i}$—Cd1—N13—C12	−37.1 (4)	N23—C24—C25—S21	−0.4 (4)
N6—Cd1—N13—C14	−37.6 (3)	C25—S21—C22—N23	1.0 (3)
$N6^{i}$—Cd1—N13—C14	143.7 (3)	C25—S21—C22—N26	179.7 (3)
N13—Cd1—S1—C2	72.66 (15)	N26—C22—N23—Cd2	−6.1 (5)
$N13^{i}$—Cd1—S1—C2	158.0 (5)	N26—C22—N23—C24	180.0 (4)

Symmetry codes: (i) $-x, y, -z+1/2$; (ii) $-x-1/2, -y+3/2, -z$.

Fig. 1


C25
S21
C22
C24
N26
S1
N23
Cd1
C2
N3
Cd2
N6
C5
S4
N13
N16
C14
C12
C15
S11