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catena-Poly[[bis[2-chloro-6-(1*H*-1,2,4-triazol-1-yl-κN^4)pyridine]cadmium(II)]-di-μ-thiocyanato-$\kappa^2 N$:*S*;$\kappa^2 S$:*N*]: a one-dimensional coordination polymer

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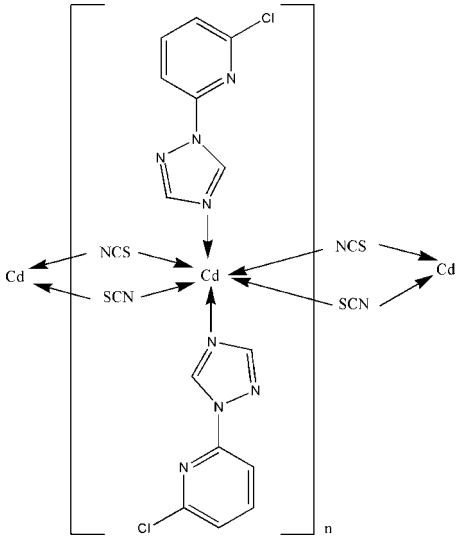
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.028; wR factor = 0.071; data-to-parameter ratio = 14.0.

In the crystal structure of the title complex, $[Cd(NCS)_2(C_7H_5ClN_4)_2]_n$, the Cd^{II} atom lies on a crystallographic inversion center and assumes a distorted octahedral geometry. The 2-chloro-6-(1*H*-1,2,4-triazol-1-yl)pyridine molecule acts as a terminal ligand. The thiocyanate ligands function as $\mu_{1,3}$-bridging units connecting adjacent Cd^{II} atoms with a separation of 5.7525 (11) Å, forming a one-dimensional chain along the *a* axis.

Related literature

For a related structure, see: Shi *et al.* (2006).



Experimental

Crystal data

$[Cd(NCS)_2(C_7H_5ClN_4)_2]$
M_r = 589.76
Triclinic, $P\overline{1}$
a = 5.7525 (11) Å
b = 8.0180 (15) Å
c = 12.212 (2) Å
α = 107.609 (3)°
β = 90.095 (2)°
γ = 91.950 (3)°
V = 536.53 (18) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.49 mm^{-1}
T = 298 (2) K
0.23 × 0.21 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.726, T_{max} = 0.865
2892 measured reflections
2005 independent reflections
1903 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.071
S = 1.03
2005 reflections
143 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N5	2.319 (2)	Cd1—S1^{i}	2.7696 (9)
Cd1—N1	2.328 (2)		
N5^{ii}—Cd1—N1	89.51 (9)	N1—Cd1—S1^{i}	90.02 (6)
N5—Cd1—N1	90.49 (9)	N5—Cd1—S1^{iii}	91.29 (7)
N5—Cd1—S1^{i}	88.71 (7)	N1—Cd1—S1^{iii}	89.98 (6)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2339).

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.* A**64**, 112–122.
Shi, J. M., Sun, Y. M., Liu, Z., Liu, L. D., Shi, W. & Cheng, P. (2006). *Dalton Trans.* pp. 376–380.

supporting information

Acta Cryst. (2008). E**64**, m1327 [doi:10.1107/S1600536808030547]

catena-Poly[[bis[2-chloro-6-(1*H*-1,2,4-triazol-1-yl-κN^4)pyridine]cadmium(II)]-di-μ-thiocyanato-κ^2N:*S*;κ^2S:*N*]: a one-dimensional coordination polymer

Zhong Nian Yang and Ting Ting Sun

S1. Comment

For a long time, thiocyanate anion has been used as a bridge ligand and a number of complexes with it have been published (Shi *et al.*, 2006). But complex dealing with 2-chloro-6-(1*H*-1,2,4-triazol-1-yl)pyridine as a ligand has not been reported as yet as our knowledge. The interest in complexes with mixed bridge ligands resulted in us synthesizing the title complex and here we report its crystal structure, (I).

The asymmetric unit and symmetry-related fragments of (I) are shown in Fig. 1. Atom Cd1 is located on an inversion center and is in a distorted octahedral CdN_4S_2 coordination geometry (Table 1). In the crystal 2-chloro-6-(1*H*-1,2,4-triazol-1-yl)pyridine molecule only acts as a unidentate terminal ligand, and thiocyanate anion functions as a μ-1,3 bridge ligand and joins a pair of Cd^{II} ions with separation of 5.7525 (11) Å. In this way a one-dimensional chain along *a* axis was fabricated as shown in Fig. 2. In addition, there is a weak π-π stacking interaction involving symmetry related 2-chloro-6-(1*H*-1,2,4-triazol-1-yl)pyridine molecules, with relevant distances being $Cg1\cdots Cg2^{i}$ = 3.7095 (19) Å, $Cg1\cdots Cg2^{i}_{perp}$ = 3.427 Å, α = 4.24° [symmetry code: (i) -*x*, 2-*y*,1-*z*; *Cg*1 and *Cg*2 are the centroids of the pyrazole ring and pyridyl ring, respectively; $Cg1\cdots Cg2^{i}_{perp}$ is the perpendicular distance from ring *Cg*1 to ring $Cg2^{i}$; α is the dihedral angle between plane *Cg*1 and plane $Cg2^{i}$.

S2. Experimental

15 ml H_2O solution containing $Cd(ClO_4)_2.6H_2O$ (0.1507 g, 0.359 mmol) and NaSCN (0.0591 g, 0.729 mmol) was added into 15 ml methanol solution of 2-chloro-6-(1*H*-1,2,4-triazol-1-yl)pyridine (0.1203 g, 0.666 mmol), and the mixed solution was stirred for a few minutes. The colorless single crystals were obtained after the filtrate had been allowed to stand at room temperature for about three weeks.

S3. Refinement

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

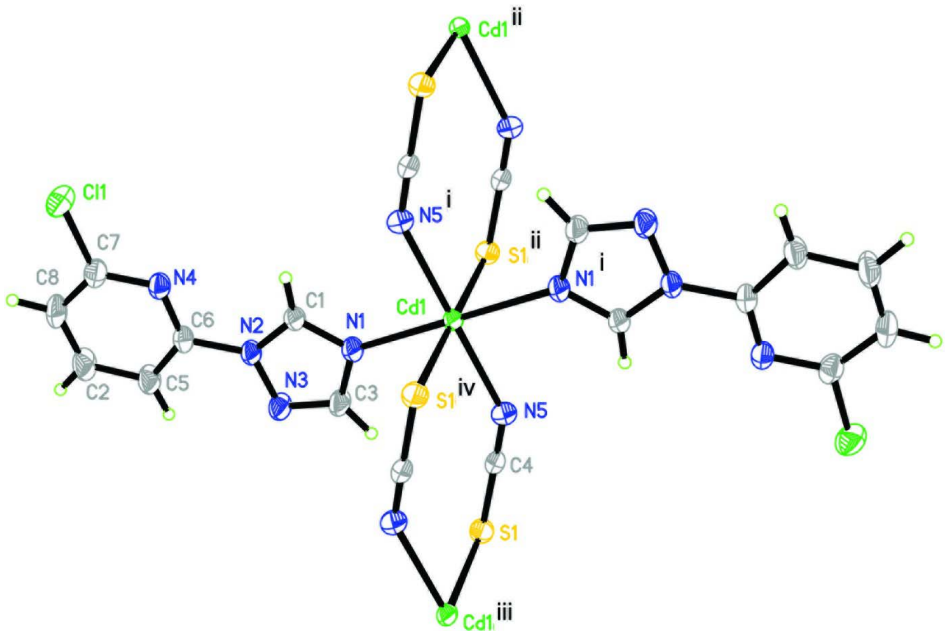

Figure 1

View of complex (I), showing the atom numbering scheme with displacement ellipsoids drawn at the 30% probability level [symmetry codes: (i) -*x*, -*y* + 2, -*z* + 2; (ii) *x* - 1, *y*, -*z* + 1; (iii) *x* + 1, *y*, *z*; (iv) -*x* + 1, -*y* + 2, -*z* + 2].

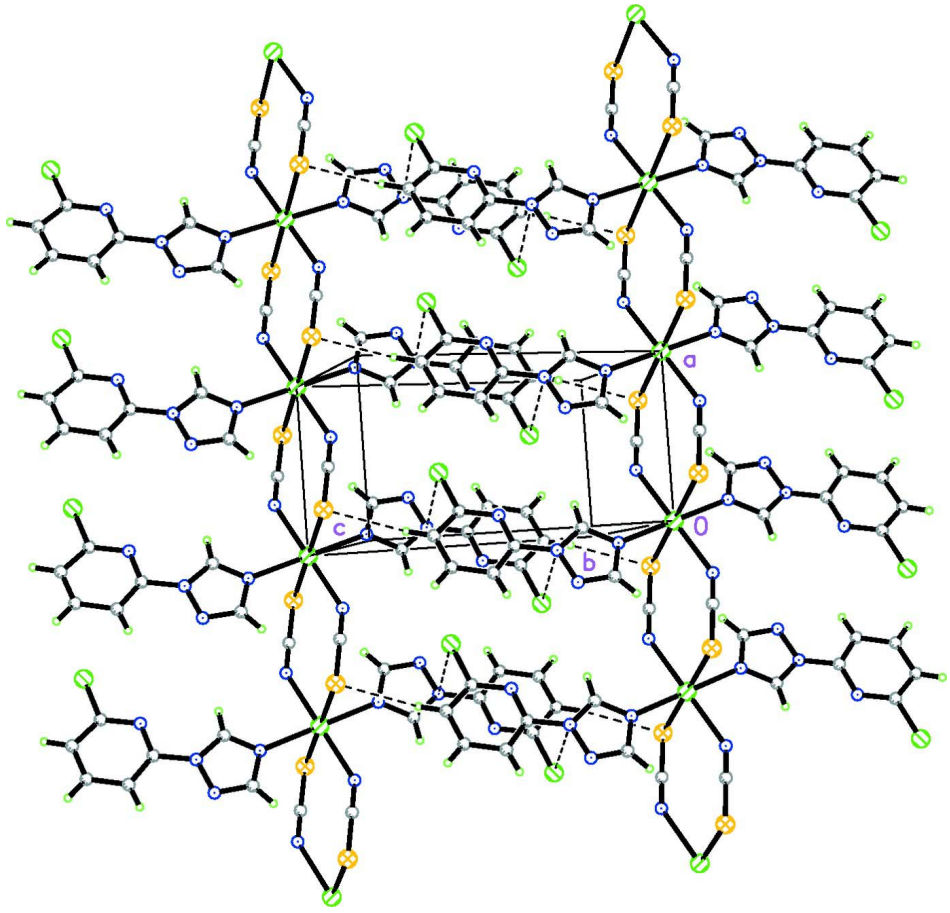

Figure 2

Packing diagram of (I), showing one-dimensional chains.

catena-Poly[[bis[2-chloro-6-(1*H*-1,2,4-triazol-1-yl- κN^4)pyridine]cadmium(II)]-di-μ-thiocyanato-κ^2N:S;κ^2S:N]

Crystal data

$[Cd(NCS)_2(C_7H_5ClN_4)_2]$
$M_r = 589.76$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.7525$ (11) Å
$b = 8.0180$ (15) Å
$c = 12.212$ (2) Å
$\alpha = 107.609$ (3)°
$\beta = 90.095$ (2)°
$\gamma = 91.950$ (3)°
$V = 536.53$ (18) Å^3
$Z = 1$
$F(000) = 290$
$D_x = 1.825$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1921 reflections
$\theta = 2.7$–28.1°
$\mu = 1.49$ mm^{-1}
$T = 298$ K
Block, colorless
0.23 × 0.21 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.726$, $T_{max} = 0.865$
2892 measured reflections
2005 independent reflections
1903 reflections with $I > 2\sigma(I)$

R_{int} = 0.016
θ_{max} = 25.8°, θ_{min} = 1.8°
h = −6→7
k = −9→8
l = −11→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.071
S = 1.03
2005 reflections
143 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
$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.1572P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.021 (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.

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}
C1	−0.0042 (5)	0.8697 (4)	0.7162 (2)	0.0411 (6)
H1	−0.1436	0.8065	0.7139	0.049*
C2	0.1609 (7)	0.7193 (5)	0.3111 (3)	0.0639 (9)
H2	0.2549	0.7310	0.2518	0.077*
C3	0.2948 (5)	1.0298 (4)	0.7697 (2)	0.0534 (8)
H3	0.4058	1.1035	0.8178	0.064*
C4	0.5043 (5)	1.2276 (4)	1.0409 (2)	0.0421 (6)
C5	0.2157 (6)	0.8143 (4)	0.4239 (2)	0.0543 (8)
H5	0.3444	0.8913	0.4426	0.065*
C6	0.0695 (5)	0.7883 (3)	0.5063 (2)	0.0406 (6)
C7	−0.1629 (6)	0.5969 (4)	0.3779 (2)	0.0484 (7)
C8	−0.0303 (7)	0.6092 (4)	0.2872 (2)	0.0597 (8)
H8	−0.0696	0.5446	0.2121	0.072*
Cd1	0.0000	1.0000	1.0000	0.04300 (14)
Cl1	−0.40595 (17)	0.45711 (12)	0.35184 (8)	0.0709 (3)
N1	0.1037 (4)	0.9656 (3)	0.81047 (18)	0.0446 (5)
N2	0.1161 (4)	0.8768 (3)	0.62460 (17)	0.0401 (5)
N3	0.3112 (4)	0.9806 (3)	0.65819 (19)	0.0530 (6)
N4	−0.1181 (4)	0.6839 (3)	0.48723 (18)	0.0420 (5)
N5	0.3274 (4)	1.1798 (4)	1.0652 (2)	0.0538 (6)

S1	0.75769 (13)	1.29435 (10)	1.00393 (6)	0.0488 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0387 (14)	0.0535 (15)	0.0288 (12)	−0.0045 (11)	0.0033 (10)	0.0098 (11)
C2	0.081 (2)	0.078 (2)	0.0301 (15)	−0.0033 (18)	0.0091 (14)	0.0133 (14)
C3	0.0507 (17)	0.073 (2)	0.0300 (13)	−0.0198 (15)	0.0021 (12)	0.0083 (13)
C4	0.0382 (15)	0.0524 (16)	0.0289 (12)	−0.0036 (12)	−0.0049 (10)	0.0026 (11)
C5	0.065 (2)	0.0628 (19)	0.0318 (14)	−0.0065 (15)	0.0078 (13)	0.0112 (13)
C6	0.0517 (16)	0.0411 (14)	0.0278 (12)	0.0034 (12)	0.0011 (11)	0.0084 (10)
C7	0.0575 (18)	0.0419 (15)	0.0413 (15)	0.0064 (12)	−0.0075 (13)	0.0052 (11)
C8	0.083 (2)	0.0602 (19)	0.0292 (14)	0.0067 (17)	−0.0040 (14)	0.0025 (13)
Cd1	0.02956 (18)	0.0703 (2)	0.02358 (16)	−0.01005 (12)	0.00224 (10)	0.00706 (12)
Cl1	0.0652 (6)	0.0672 (5)	0.0659 (5)	−0.0086 (4)	−0.0153 (4)	0.0000 (4)
N1	0.0437 (13)	0.0585 (14)	0.0279 (11)	−0.0047 (10)	0.0042 (9)	0.0085 (10)
N2	0.0434 (13)	0.0482 (12)	0.0263 (10)	−0.0039 (10)	0.0034 (9)	0.0082 (9)
N3	0.0533 (15)	0.0698 (16)	0.0312 (12)	−0.0195 (12)	0.0052 (10)	0.0105 (11)
N4	0.0487 (14)	0.0434 (12)	0.0321 (11)	0.0048 (10)	−0.0018 (9)	0.0084 (9)
N5	0.0360 (14)	0.0676 (16)	0.0479 (14)	−0.0086 (11)	0.0004 (10)	0.0035 (12)
S1	0.0407 (4)	0.0620 (5)	0.0401 (4)	−0.0104 (3)	0.0037 (3)	0.0113 (3)

Geometric parameters (Å, º)

C1—N1	1.316 (3)	C6—N2	1.425 (3)
C1—N2	1.331 (3)	C7—N4	1.326 (3)
C1—H1	0.9300	C7—C8	1.372 (5)
C2—C8	1.361 (5)	C7—Cl1	1.729 (3)
C2—C5	1.387 (4)	C8—H8	0.9300
C2—H2	0.9300	Cd1—N5^{i}	2.319 (2)
C3—N3	1.303 (3)	Cd1—N5	2.319 (2)
C3—N1	1.356 (3)	Cd1—N1	2.328 (2)
C3—H3	0.9300	Cd1—N1^{i}	2.328 (2)
C4—N5	1.146 (4)	Cd1—S1^{ii}	2.7696 (9)
C4—S1	1.646 (3)	Cd1—S1^{iii}	2.7696 (9)
C5—C6	1.371 (4)	N2—N3	1.360 (3)
C5—H5	0.9300	S1—Cd1^{iv}	2.7696 (9)
C6—N4	1.319 (4)		
N1—C1—N2	109.8 (2)	N5—Cd1—N1	90.49 (9)
N1—C1—H1	125.1	N5^{i}—Cd1—N1^{i}	90.49 (9)
N2—C1—H1	125.1	N5—Cd1—N1^{i}	89.51 (9)
C8—C2—C5	120.1 (3)	N1—Cd1—N1^{i}	180.000 (1)
C8—C2—H2	120.0	N5^{i}—Cd1—S1^{ii}	91.29 (7)
C5—C2—H2	120.0	N5—Cd1—S1^{ii}	88.71 (7)
N3—C3—N1	115.0 (3)	N1—Cd1—S1^{ii}	90.02 (6)
N3—C3—H3	122.5	N1^{i}—Cd1—S1^{ii}	89.98 (6)
N1—C3—H3	122.5	N5^{i}—Cd1—S1^{iii}	88.71 (7)

N5—C4—S1	179.1 (3)	N5—Cd1—S1^{iii}	91.29 (7)
C6—C5—C2	116.3 (3)	N1—Cd1—S1^{iii}	89.98 (6)
C6—C5—H5	121.9	N1^{i}—Cd1—S1^{iii}	90.02 (6)
C2—C5—H5	121.9	S1^{ii}—Cd1—S1^{iii}	180.0
N4—C6—C5	125.8 (3)	C1—N1—C3	103.0 (2)
N4—C6—N2	114.1 (2)	C1—N1—Cd1	127.88 (18)
C5—C6—N2	120.1 (3)	C3—N1—Cd1	129.05 (18)
N4—C7—C8	124.9 (3)	C1—N2—N3	110.0 (2)
N4—C7—Cl1	115.9 (2)	C1—N2—C6	129.0 (2)
C8—C7—Cl1	119.2 (2)	N3—N2—C6	120.9 (2)
C2—C8—C7	117.6 (3)	C3—N3—N2	102.2 (2)
C2—C8—H8	121.2	C6—N4—C7	115.4 (2)
C7—C8—H8	121.2	C4—N5—Cd1	145.7 (2)
N5^{i}—Cd1—N5	180.0	C4—S1—Cd1^{iv}	97.18 (11)
N5^{i}—Cd1—N1	89.51 (9)		

C8—C2—C5—C6	0.6 (5)	N1—C1—N2—N3	0.1 (3)
C2—C5—C6—N4	−1.0 (5)	N1—C1—N2—C6	177.3 (3)
C2—C5—C6—N2	178.3 (3)	N4—C6—N2—C1	−1.0 (4)
C5—C2—C8—C7	0.0 (5)	C5—C6—N2—C1	179.6 (3)
N4—C7—C8—C2	−0.3 (5)	N4—C6—N2—N3	175.9 (2)
Cl1—C7—C8—C2	−179.4 (3)	C5—C6—N2—N3	−3.5 (4)
N2—C1—N1—C3	−0.1 (3)	N1—C3—N3—N2	−0.1 (4)
N2—C1—N1—Cd1	−176.61 (18)	C1—N2—N3—C3	0.0 (3)
N3—C3—N1—C1	0.1 (4)	C6—N2—N3—C3	−177.5 (3)
N3—C3—N1—Cd1	176.6 (2)	C5—C6—N4—C7	0.8 (4)
N5^{i}—Cd1—N1—C1	−1.9 (3)	N2—C6—N4—C7	−178.6 (2)
N5—Cd1—N1—C1	178.1 (3)	C8—C7—N4—C6	−0.1 (4)
S1^{ii}—Cd1—N1—C1	−93.2 (2)	Cl1—C7—N4—C6	179.1 (2)
S1^{iii}—Cd1—N1—C1	86.8 (2)	N1—Cd1—N5—C4	−14.4 (5)
N5^{i}—Cd1—N1—C3	−177.6 (3)	N1^{i}—Cd1—N5—C4	165.6 (5)
N5—Cd1—N1—C3	2.4 (3)	S1^{ii}—Cd1—N5—C4	−104.4 (4)
S1^{ii}—Cd1—N1—C3	91.1 (3)	S1^{iii}—Cd1—N5—C4	75.6 (4)
S1^{iii}—Cd1—N1—C3	−88.9 (3)		

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