IUCrData

ISSN 2414-3146

catena-Poly[[chloridotris(1,3-thiazolidine-2-thione-κS)cadmium(II)]-μ-chlorido]

Aboubacar Diop,[a]* Tidiane Diop,[a] Antoine Blaise Kama,[a] Cheikh Abdou Khadre Diop[a] and Nikolay Tumanov[b]

[a]Laboratoire de Chimie Minérale et Analytique (LA.CHI.MI.A), Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, and [b]Departement de Chimie, Université de Namur, Rue de Bruxelles 61-5000, Namur, Belgium. *Correspondence e-mail: aboubacar.diop@ucad.edu.sn

Received 8 October 2020
Accepted 26 October 2020

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

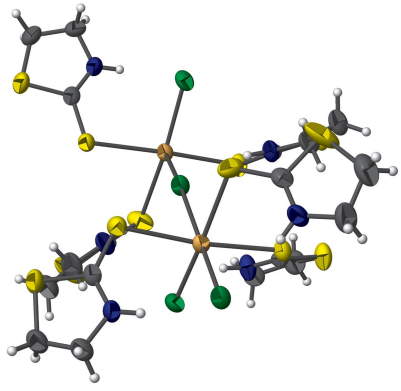
Keywords: crystal structure; 1,3-thiazolidine-2-thione; cadmium centre; hydrogen bonding.

CCDC reference: 2040604

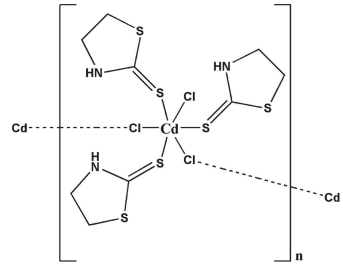
Structural data: full structural data are available from iucrdata.iucr.org

The synthesis and characterization of poly[dichloridotri(1,3-thiazolidine-2-thione)cadmium(II)], $[CdCl_2(C_3H_5NS_2)_3]_n$, prepared from $CdCl_2{\cdot}H_2O$ and $C_3H_5NS_2$ (tzdSH) in a 1:3 ratio, are described. The Cd^{II} cation is coordinated by three 1,3-thiazolidine-2-thione molecules and three Cl^- anions in a distorted octahedral environment. The Cd metal centres are connected *via* Cl^- ligands, creating polymeric chains running along the *a*-axis direction. The conformation of the chains is stabilized by N—H···Cl hydrogen bonds.

3D view



Chemical scheme



Structure description

1,3-Thiazolidine-2-thione (tzdSH: $C_3H_5NS_2$), is a well-known heterocyclic thione/thiol ligand. Crystallographic studies and investigations of its modes of coordination have been reported (Saithong *et al.*, 2007). We are interested in the coordination behaviour and structure of tzdSH complexes with Cd^{II} chloride. The synthesis is accompanied by a transformation of the tzdSH (tzdSH: $C_3H_5NS_2$, thiol form) into a tzdt ligand (tzdt: $C_3H_5NS_2$, thion form). A similar transformation was described previously by Saithong *et al.* (2014). Metal complexes of thiones and thionates were reviewed by Raper (1997).

Cadmium (II) is known to form a wide variety of 1:1 to 1:4 complexes with thiones, where the structural arrangements are generally tetrahedral and octahedral coordination environments (Mahmood *et al.*, 2018). The 1:1 complexes, for example [Cd(Melmt)-(S_eCN)] (Melmt = *N*-methylimidazolidine-2-thione; Fettouhi *et al.*, 2008) usually exist in the polymeric form. The 1:2 complexes such as $[Cd(Dmtu)_2X_2]$ (Dmtu = *N*,*N*′-dimethylthiourea-κS; *X* = Cl, Br, I; Ahmad *et al.*, 2011) are the most common and often consist of discrete monomeric molecules with a terahedrally (Moloto *et al.*, 2003) or octahedrally (Mahmood *et al.*, 2012) coordinated Cd^{II} ion. The 1:3 compounds are rare:

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{i}	0.86	2.43	3.260 (4)	163
N2—H2···Cl1^{i}	0.86	2.47	3.314 (4)	168
N3—H3···Cl2	0.86	2.41	3.165 (4)	147
C8—H8B···Cl1^{ii}	0.97	2.82	3.781 (6)	171

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

the structure of $[Cd(Tu)_3(SO_4)]$ shows that the complex is a dimer, and the coordination around the metal atom is intermediate between square pyramidal and trigonal bipyramidal (Corao & Baggio, 1969). The 1:4 complexes may be ionic or non-ionic (Mahmood *et al.*, 2018).

The above structural studies show that thiones coordinate to cadmium (II) *via* the sulfur atom. To further investigate the structural aspects of such complexes, we report in this work a complex with a Cd^{II}:thione ratio of 1:23. The asymmetric unit consists of a cadmium (II) ion bonded to three 1,3-thiazolidine-2-thione moieties *via* the exocyclic sulfur atom and two Cl atoms (Fig. 1). The Cd—S and Cd—Cl bond lengths are in the range 2.7004 (11)–2.7347 (13) and 2.5430 (12)–2.7258 (16) Å, respectively. The bond lengths are slightly different from those reported in the literature [Cd—S = 2.604 Å and Cd—Cl = 2.7105 Å; Bell *et al.*, 2004]. This may be due to the intramolecular hydrogen bonds observed in the crystal structure.

In the crystal, one of Cl^- anions connects two neighbouring Cd^{II} centers leading to polymeric chains. No hydrogen bonds are observed between the chains. The structure of the compound can be described as parallel chains running along the *a*-axis direction. The conformation of the chains is stabilized by N—H···Cl hydrogen bonds (Table 1, Fig. 2).

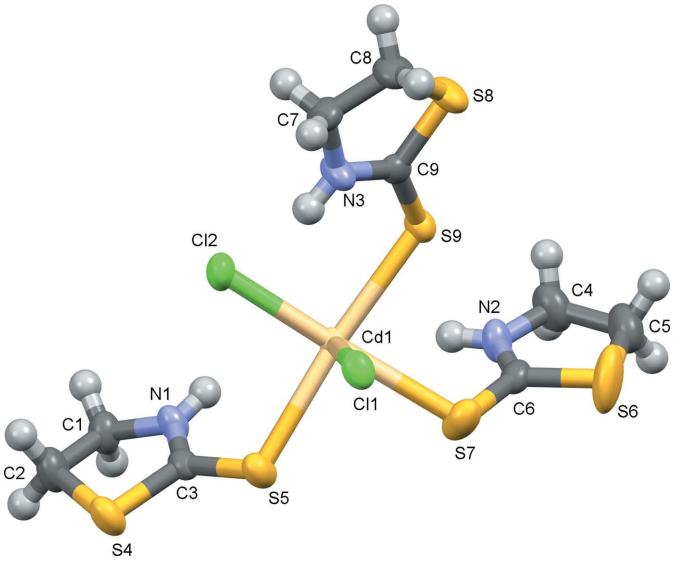


Figure 1
The asymmetric unit of title compound with displacement ellipsoids drawn at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CdCl_2(C_3H_5NS_2)_3]$
M_r	540.90
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	295
a, b, c (Å)	9.2014 (3), 19.3472 (6), 10.5827 (3)
V (Å^3)	1883.94 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.10
Crystal size (mm)	0.76 × 0.50 × 0.14
Data collection	
Diffractometer	Oxford Diffraction Xcalibur, Ruby, Gemini Ultra
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2018)
T_{min}, T_{max}	0.242, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12033, 5594, 4781
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.069, 1.01
No. of reflections	5594
No. of parameters	190
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.79
Absolute structure	Flack x determined using 1872 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.010 (19)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015*a*) and *SHELXL2018/3* (Sheldrick, 2015*b*).

Synthesis and crystallization

In a round-bottom flask, to the ligand (tzdSH: $C_3H_5NS_2$) (15 mmol, 1.79 g) in 5 mL of 1,4-dioxan, a solution of $CdCl_2{\cdot}H_2O$ (5 mmol, 1.01 g) in 5 mL of distilled water was added. The mixture was refluxed for 4 h. Light-yellow crystals

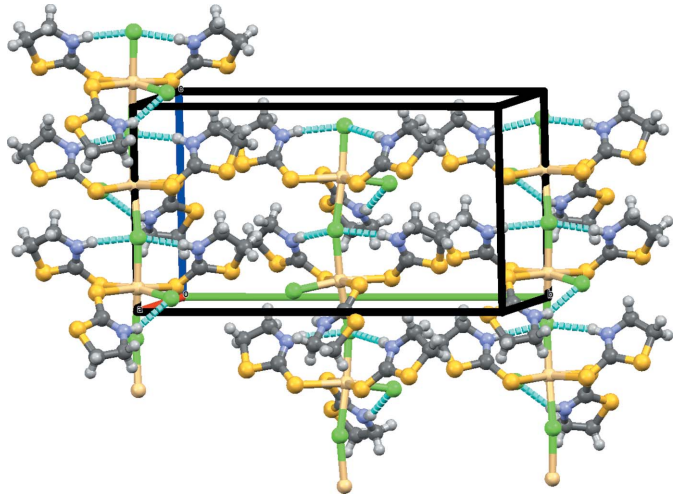


Figure 2
Packing diagram of the title compound. N—H···Cl hydrogen bonds are show as light blue dashed lines.

appeared after the light yellow filtrate had been kept at room temperature for two days (yield 75%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the crystallographic service of Chemistry Department of Namur University (Belgium) for the data collection.

Funding information

The authors acknowledge the Cheikh Anta Diop University of Dakar (Senegal) for financial support.

References

Ahmad, S., Altaf, M., Stoeckli-Evans, H., Isab, M. R., Malik, M. R., Ali, S. & Shuja, S. (2011). *J. Chem. Crystallogr.* **41**, 1099–1104.
Bell, N. A., Clegg, W., Coles, S. J., Constable, C. P., Harrington, R. W., Hursthouse, M. B., Light, M. E., Raper, E. S., Sammon, C. & Walker, M. R. (2004). *Inorg. Chim. Acta*, **357**, 2091–2099.
Corao, E. & Baggio, S. (1969). *Inorg. Chim. Acta*, **3**, 617–622.
Fettouhi, M., Wazeer, M. I. M. & Isab, A. A. (2008). *Inorg. Chem. Commun.* **11**, 252–255.
Mahmood, R., Ahmad, S., Fettouhi, M., Roisnel, T., Gilani, M. A., Mehmood, K., Murtaza, G. & Isab, A. A. (2018). *J. Mol. Struct.* **1156**, 235–242.
Mahmood, R., Ghulam Hussain, S., Fettouhi, M., Isab, A. A. & Ahmad, S. (2012). *Acta Cryst.* E**68**, m1352–m1353.
Moloto, M. J., Malik, M. A., O'Brien, P., Motevalli, M. & Kolawole, G. A. (2003). *Polyhedron*, **22**, 595–603.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Raper, E. S. (1997). *Coord. Chem. Rev.* **165**, 475–567.
Rigaku OD (2018). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Saithong, S., Klongkleaw, P., Pakawatchai, C. & Mokakul, J. (2014). *Acta Cryst.* E**70**, 90–93.
Saithong, S., Pakawatchai, C. & Charmant, J. P. H. (2007). *Acta Cryst.* E**63**, m857–m858.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2020). **5**, x201423 [https://doi.org/10.1107/S2414314620014236]

catena-Poly[[chloridotris(1,3-thiazolidine-2-thione-κ*S*)cadmium(II)]-μ-chlorido]

Aboubacar Diop, Tidiane Diop, Antoine Blaise Kama, Cheikh Abdou Khadre Diop and Nikolay Tumanov

***catena*-Poly[[chloridotris(1,3-thiazolidine-2-thione-κ*S*)cadmium(II)]-μ-chlorido]**

Crystal data

$[CdCl_2(C_3H_5NS_2)_3]$
M_r = 540.90
Orthorhombic, $Pna2_1$
a = 9.2014 (3) Å
b = 19.3472 (6) Å
c = 10.5827 (3) Å
V = 1883.94 (9) Å^3
Z = 4
$F(000)$ = 1072
D_x = 1.907 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4396 reflections
θ = 3.1–32.5°
μ = 2.10 mm^{-1}
T = 295 K
Block, colourless
0.76 × 0.50 × 0.14 mm

Data collection

Oxford Diffraction Xcalibur, Ruby, Gemini Ultra diffractometer
Graphite monochromator
Detector resolution: 10.3712 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2018)
T_{min} = 0.242, T_{max} = 1.000
12033 measured reflections
5594 independent reflections
4781 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.5°, θ_{min} = 2.1°
h = −12→13
k = −27→27
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.069
S = 1.01
5594 reflections
190 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: dual
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack x determined using 1872 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.010 (19)

Special details

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

Refinement. H atoms were refined using a riding model with N—H = 0.86 Å or C—H = 0.97 Å and U(H)=1.2U_{eq}(C,*N*).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	−0.51629 (3)	−0.49641 (2)	−0.38259 (5)	0.03293 (9)
Cl1	−0.46306 (13)	−0.51075 (6)	−0.63461 (14)	0.0402 (3)
Cl2	−0.66097 (13)	−0.38657 (6)	−0.42258 (12)	0.0459 (3)
S4	−0.17107 (15)	−0.28169 (7)	−0.32587 (13)	0.0514 (3)
S5	−0.26212 (12)	−0.42407 (7)	−0.39534 (14)	0.0470 (3)
S6	−0.4464 (3)	−0.76006 (9)	−0.31381 (18)	0.0922 (7)
S7	−0.36450 (15)	−0.61793 (7)	−0.38167 (16)	0.0594 (4)
S8	−1.01474 (16)	−0.59987 (9)	−0.54807 (18)	0.0592 (4)
S9	−0.75414 (11)	−0.57811 (6)	−0.38890 (14)	0.0401 (2)
N1	−0.3576 (4)	−0.3483 (2)	−0.1994 (3)	0.0415 (9)
H1	−0.420149	−0.379411	−0.179291	0.050*
N2	−0.5236 (5)	−0.6583 (2)	−0.1835 (4)	0.0483 (11)
H2	−0.532251	−0.616145	−0.158878	0.058*
N3	−0.8589 (5)	−0.4936 (2)	−0.5693 (4)	0.0515 (12)
H3	−0.786934	−0.465732	−0.559655	0.062*
C1	−0.3397 (6)	−0.2853 (3)	−0.1234 (5)	0.0504 (13)
H1A	−0.282523	−0.295177	−0.048554	0.061*
H1B	−0.433815	−0.267960	−0.097001	0.061*
C2	−0.2647 (6)	−0.2334 (3)	−0.2030 (5)	0.0574 (14)
H2A	−0.195748	−0.207054	−0.153008	0.069*
H2B	−0.334355	−0.201629	−0.239964	0.069*
C3	−0.2750 (5)	−0.3550 (2)	−0.2982 (4)	0.0352 (10)
C4	−0.5903 (8)	−0.7138 (3)	−0.1123 (6)	0.0678 (18)
H4A	−0.695161	−0.708523	−0.112475	0.081*
H4B	−0.556857	−0.712710	−0.025382	0.081*
C5	−0.5487 (8)	−0.7815 (3)	−0.1731 (6)	0.075 (2)
H5A	−0.634932	−0.807737	−0.194980	0.090*
H5B	−0.489916	−0.808860	−0.115812	0.090*
C6	−0.4508 (5)	−0.6730 (3)	−0.2845 (4)	0.0403 (11)
C7	−0.9747 (5)	−0.4783 (3)	−0.6584 (6)	0.0509 (14)
H7A	−0.934127	−0.462911	−0.738207	0.061*
H7B	−1.036634	−0.441940	−0.625452	0.061*
C8	−1.0607 (6)	−0.5430 (3)	−0.6772 (6)	0.0596 (16)
H8A	−1.035978	−0.564345	−0.757395	0.072*
H8B	−1.163928	−0.532937	−0.676816	0.072*
C9	−0.8670 (5)	−0.5509 (3)	−0.5041 (4)	0.0356 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04166 (16)	0.03310 (15)	0.02402 (13)	−0.00411 (12)	0.0009 (2)	−0.00111 (16)
Cl1	0.0570 (9)	0.0418 (7)	0.0218 (4)	−0.0097 (5)	0.0013 (7)	−0.0008 (6)
Cl2	0.0537 (6)	0.0311 (6)	0.0529 (7)	0.0001 (5)	0.0046 (5)	−0.0039 (5)
S4	0.0563 (7)	0.0483 (8)	0.0496 (6)	−0.0205 (7)	0.0097 (6)	−0.0042 (7)
S5	0.0468 (6)	0.0463 (7)	0.0478 (7)	−0.0101 (5)	0.0080 (6)	−0.0116 (7)
S6	0.175 (2)	0.0366 (8)	0.0653 (9)	0.0215 (12)	0.0102 (13)	−0.0082 (8)
S7	0.0625 (7)	0.0549 (8)	0.0609 (8)	0.0190 (7)	0.0232 (9)	0.0123 (9)
S8	0.0489 (8)	0.0566 (10)	0.0720 (9)	−0.0200 (7)	−0.0169 (7)	0.0102 (8)
S9	0.0440 (5)	0.0367 (5)	0.0396 (5)	−0.0068 (4)	−0.0045 (6)	0.0030 (7)
N1	0.049 (2)	0.037 (2)	0.038 (2)	−0.012 (2)	0.0054 (18)	−0.0005 (18)
N2	0.070 (3)	0.034 (2)	0.041 (2)	−0.005 (2)	0.006 (2)	−0.0051 (19)
N3	0.048 (3)	0.045 (3)	0.062 (3)	−0.014 (2)	−0.018 (2)	0.011 (2)
C1	0.068 (3)	0.039 (3)	0.044 (3)	−0.002 (3)	0.003 (3)	−0.003 (3)
C2	0.075 (4)	0.042 (3)	0.056 (3)	−0.011 (3)	0.007 (3)	−0.010 (3)
C3	0.037 (2)	0.036 (2)	0.033 (2)	−0.005 (2)	−0.0081 (18)	0.0030 (19)
C4	0.085 (5)	0.058 (4)	0.060 (4)	−0.021 (4)	0.005 (3)	0.006 (3)
C5	0.092 (5)	0.047 (4)	0.087 (5)	−0.011 (4)	−0.014 (4)	0.010 (4)
C6	0.044 (2)	0.036 (3)	0.041 (3)	0.007 (2)	−0.008 (2)	−0.001 (2)
C7	0.047 (3)	0.049 (3)	0.057 (4)	0.009 (3)	−0.013 (3)	0.005 (3)
C8	0.044 (3)	0.064 (4)	0.071 (4)	−0.003 (3)	−0.021 (3)	0.002 (3)
C9	0.034 (2)	0.037 (3)	0.036 (2)	0.001 (2)	0.0045 (17)	−0.0071 (19)

Geometric parameters (Å, º)

Cd1—Cl2	2.5430 (12)	N2—H2	0.8600
Cd1—Cl1^{i}	2.6348 (16)	N3—C9	1.307 (6)
Cd1—S9	2.7004 (11)	N3—C7	1.454 (7)
Cd1—Cl1	2.7258 (16)	N3—H3	0.8600
Cd1—S5	2.7289 (12)	C1—C2	1.482 (7)
Cd1—S7	2.7347 (13)	C1—H1A	0.9700
S4—C3	1.736 (5)	C1—H1B	0.9700
S4—C2	1.818 (5)	C2—H2A	0.9700
S5—C3	1.690 (5)	C2—H2B	0.9700
S6—C6	1.714 (5)	C4—C5	1.509 (9)
S6—C5	1.810 (7)	C4—H4A	0.9700
S7—C6	1.679 (5)	C4—H4B	0.9700
S8—C9	1.721 (5)	C5—H5A	0.9700
S8—C8	1.804 (6)	C5—H5B	0.9700
S9—C9	1.686 (5)	C7—C8	1.495 (9)
N1—C3	1.299 (5)	C7—H7A	0.9700
N1—C1	1.469 (6)	C7—H7B	0.9700
N1—H1	0.8600	C8—H8A	0.9700
N2—C6	1.293 (6)	C8—H8B	0.9700
N2—C4	1.448 (7)		

Cl2—Cd1—Cl1^{i}	94.82 (4)	C1—C2—H2A	110.5
Cl2—Cd1—S9	93.48 (4)	S4—C2—H2A	110.5
Cl1^{i}—Cd1—S9	89.83 (4)	C1—C2—H2B	110.5
Cl2—Cd1—Cl1	90.94 (4)	S4—C2—H2B	110.5
Cl1^{i}—Cd1—Cl1	173.143 (17)	H2A—C2—H2B	108.7
S9—Cd1—Cl1	93.55 (4)	N1—C3—S5	127.6 (4)
Cl2—Cd1—S5	90.68 (4)	N1—C3—S4	112.1 (4)
Cl1^{i}—Cd1—S5	94.82 (4)	S5—C3—S4	120.3 (3)
S9—Cd1—S5	173.48 (5)	N2—C4—C5	108.3 (5)
Cl1—Cd1—S5	81.36 (4)	N2—C4—H4A	110.0
Cl2—Cd1—S7	170.53 (6)	C5—C4—H4A	110.0
Cl1^{i}—Cd1—S7	94.51 (5)	N2—C4—H4B	110.0
S9—Cd1—S7	84.88 (4)	C5—C4—H4B	110.0
Cl1—Cd1—S7	79.87 (5)	H4A—C4—H4B	108.4
S5—Cd1—S7	90.19 (4)	C4—C5—S6	106.5 (4)
Cd1^{ii}—Cl1—Cd1	162.98 (5)	C4—C5—H5A	110.4
C3—S4—C2	92.2 (2)	S6—C5—H5A	110.4
C3—S5—Cd1	108.37 (16)	C4—C5—H5B	110.4
C6—S6—C5	93.7 (3)	S6—C5—H5B	110.4
C6—S7—Cd1	107.80 (17)	H5A—C5—H5B	108.6
C9—S8—C8	93.1 (3)	N2—C6—S7	127.7 (4)
C9—S9—Cd1	109.53 (18)	N2—C6—S6	112.2 (4)
C3—N1—C1	117.3 (4)	S7—C6—S6	120.1 (3)
C3—N1—H1	121.4	N3—C7—C8	107.7 (5)
C1—N1—H1	121.4	N3—C7—H7A	110.2
C6—N2—C4	119.2 (5)	C8—C7—H7A	110.2
C6—N2—H2	120.4	N3—C7—H7B	110.2
C4—N2—H2	120.4	C8—C7—H7B	110.2
C9—N3—C7	118.2 (5)	H7A—C7—H7B	108.5
C9—N3—H3	120.9	C7—C8—S8	106.6 (4)
C7—N3—H3	120.9	C7—C8—H8A	110.4
N1—C1—C2	107.7 (4)	S8—C8—H8A	110.4
N1—C1—H1A	110.2	C7—C8—H8B	110.4
C2—C1—H1A	110.2	S8—C8—H8B	110.4
N1—C1—H1B	110.2	H8A—C8—H8B	108.6
C2—C1—H1B	110.2	N3—C9—S9	127.7 (4)
H1A—C1—H1B	108.5	N3—C9—S8	111.7 (4)
C1—C2—S4	106.1 (4)	S9—C9—S8	120.7 (3)

C3—N1—C1—C2	18.9 (6)	Cd1—S7—C6—N2	−32.2 (5)
N1—C1—C2—S4	−21.9 (5)	Cd1—S7—C6—S6	148.6 (2)
C3—S4—C2—C1	17.1 (4)	C5—S6—C6—N2	−1.8 (4)
C1—N1—C3—S5	174.6 (4)	C5—S6—C6—S7	177.5 (3)
C1—N1—C3—S4	−5.7 (5)	C9—N3—C7—C8	−14.1 (7)
Cd1—S5—C3—N1	25.0 (4)	N3—C7—C8—S8	16.8 (6)
Cd1—S5—C3—S4	−154.7 (2)	C9—S8—C8—C7	−13.4 (4)
C2—S4—C3—N1	−7.2 (4)	C7—N3—C9—S9	−175.6 (4)
C2—S4—C3—S5	172.5 (3)	C7—N3—C9—S8	3.8 (6)

C6—N2—C4—C5	3.6 (7)	Cd1—S9—C9—N3	−10.5 (5)
N2—C4—C5—S6	−4.4 (7)	Cd1—S9—C9—S8	170.1 (2)
C6—S6—C5—C4	3.6 (5)	C8—S8—C9—N3	6.1 (4)
C4—N2—C6—S7	−180.0 (4)	C8—S8—C9—S9	−174.4 (3)
C4—N2—C6—S6	−0.8 (6)		

Symmetry codes: (i) −*x*−1, −*y*−1, *z*+1/2; (ii) −*x*−1, −*y*−1, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1^{i}	0.86	2.43	3.260 (4)	163
N2—H2···Cl1^{i}	0.86	2.47	3.314 (4)	168
N3—H3···Cl2	0.86	2.41	3.165 (4)	147
C8—H8*B*···Cl1^{iii}	0.97	2.82	3.781 (6)	171

Symmetry codes: (i) −*x*−1, −*y*−1, *z*+1/2; (iii) *x*−1, *y*, *z*.