Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[benzyltrimethylammonium [cadmium(II)-tri-μ_2-thiocyanato]]

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.041
wR factor = 0.067
Data-to-parameter ratio = 18.1

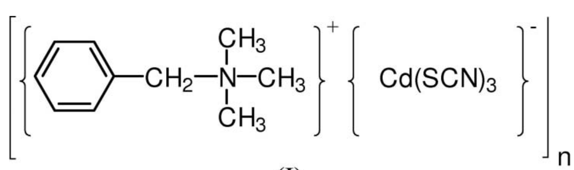
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 1 June 2006
Accepted 14 June 2006

The title compound, $\{(C_{10}H_{16}N)[Cd(SCN)_3]\}_n$, contains $[(C_6H_5CH_2)N(CH_3)_3]^+$ cations lying between one-dimensional chains of stoichiometry $\{[Cd(SCN)_3]^-\}_n$. Each Cd^{II} ion is 3*N*,3*S*-hexacoordinated by thiocyanate ligands, in an octahedral *fac* arrangement. The asymmetric unit contains two cations and two anions.

Comment

In recent years, studies of the synthesis and properties of semiconductor materials such as CdS and CdSe have become an area of interest owing to the great scope for fundamental understanding of materials as well as potential technological applications (Zhang *et al.*, 1999), such as light-emitting devices, non-linear optical devices, solar cells and biological labels. As a result, the search for new precursors, such as salts containing $[Cd(SCN)_3]^-$, is receiving much attention. As the d^{10} configuration and softness of Cd^{II} permit a wide variety of geometries and coordination numbers, especially with the ambidentate ligand thiocyanate (SCN^-), various structural types have been observed. Which structural type occurs depends on the size, shape and symmetry of the counter-cations and also on the ratio of Cd^{2+} to SCN^- ions. Thus, the structures of a number of one-dimensional single chains (Zhang *et al.*, 2001), two-dimensional networks (Zhang *et al.*, 1997) and three-dimensional structures (Thiele & Messer, 1980) have been reported and reviewed (Sun *et al.*, 2001). Of special interest are the low-dimensional structural motifs, since these relate to highly anisotropic physical properties. In continuation of our interest in the supramolecular chemistry of salts of simple metal complexes (Sharma *et al.*, 2005, 2006), the synthesis and characterization of the title compound, (I), was undertaken.



(I)

For (I), structure determination revealed the presence of four crystallographically independent components in the solid state: two $[(C_6H_5CH_2)N(CH_3)_3]^+$ cations and two $[Cd(SCN)_3]^-$ anions (Fig. 1). Each Cd^{II} ion is 3*N*,3*S*-hexacoordinated, and adopts a slightly deformed *fac* octahedral geometry. Thus, each S atom is *trans* to an N atom. One of the thiocyanate ions (S6/C6/N6) appears to be rotationally disordered about its central C atom, which modifies the Cd^{II}

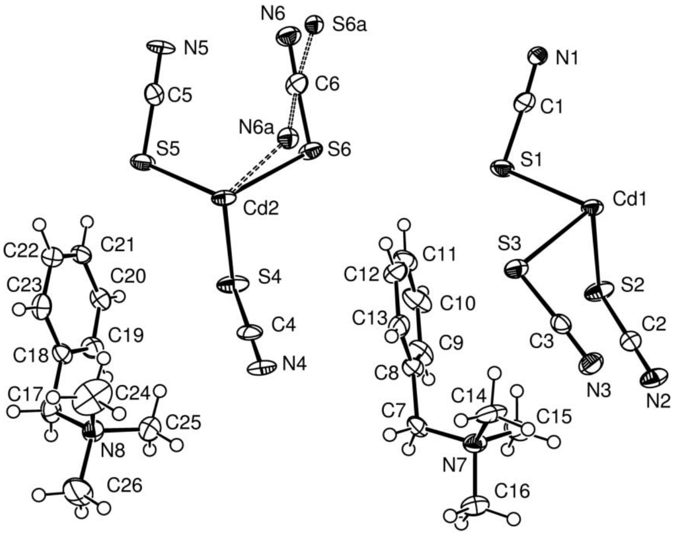


Figure 1
The contents of the asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level for non-H atoms. The minor disorder component is indicated by dashed bonds.

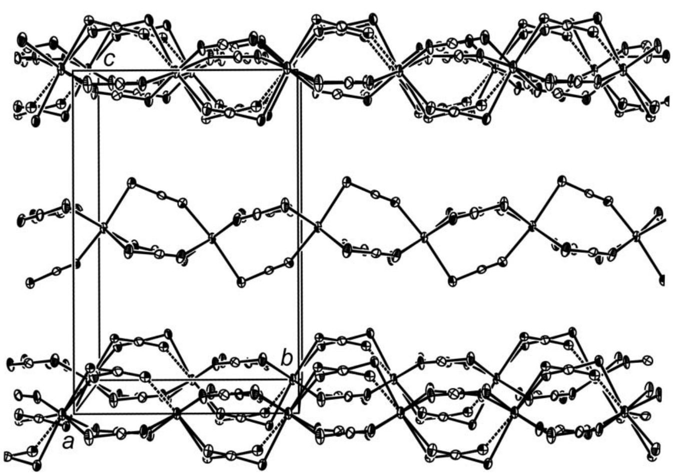


Figure 2
The polymeric $\{[Cd(SCN)_3]^-\}_n$ chains extending along the *b*-axis direction.

coordination geometry at 9% of the Cd2 metal sites. Both the Cd—S and Cd—N bond lengths show considerable variation (Table 1). Similar distances (Cd—S = 2.688–2.743 Å and Cd—N = 2.279–2.379 Å) are observed in $[(CH_3)_4N][Cd(SCN)_3]$, which is also 3*N*,3*S*-coordinated (Kuniyasu *et al.*, 1987). The average Cd—N—C and Cd—S—C angles in (I) (142.11 and 98.93°, respectively) are also comparable with those in $[(CH_3)_4N][Cd(SCN)_3]$. The $\{[Cd(SCN)_3]^-\}_n$ chains (Fig. 2) propagate along the *b*-axis direction, with $[Cd(SCN)_6]$ octahedra linked in a face-sharing manner *via* the shared SCN^- ligands. The $[(C_6H_5CH_2)N(CH_3)_3]^+$ cations occupy positions between the chains. It is generally believed that the relative arrangement of the anionic $\{[Cd(SCN)_3]^-\}_n$ chains is strongly influenced by the size and shape of the cation. With larger cations, parallel alignment of the $\{[Cd(SCN)_3]^-\}_n$ chains is expected; this is observed in (I).

Experimental

Analytical grade reagents were used without any further purification. Benzyltrimethylammonium chloride (1.0 g, 0.005 mol) was dissolved in 10 ml water, while $CdCl_2$ (0.98 g, 0.004 mol) and ammonium thiocyanate (1.22 g, 0.016 mol) were dissolved in 20 ml water by mechanical stirring. The solutions were mixed and a curd-like white solid precipitated immediately. This was filtered off and dried in air. Crystals of (I) were obtained after redissolving the white solid in an acetone–water mixture (1:1) at room temperature. The salt decomposes at 393 K and is insoluble in organic solvents (C_2H_5OH, CCl_4 and CH_3Cl), but soluble in DMSO and hot water. IR (KBr, ν, cm^{-1}): 2116 (*s*), 2087 (*s*, SCN), 1660 (*m*), 1553 (*m*), 1081 (*s*), 1028 (*s*), 1002 (*s*). ^1H NMR (d_6-DMSO, 298 K): δ 7.2 (*s*, 5H, HAr), 4.2 (*s*, 2H, $ArCH_2$), 2.6 (*s*, 9H, CH_3). ^{13}C NMR (d_6-DMSO, 298 K): δ 128–133 (Ar), 126 (SCN), 68 (ArC), 25 (CH_3).

Crystal data

$(C_{10}H_{16}N)[Cd(SCN)_3]$
$M_r = 436.88$
Monoclinic, $P2_1$
$a = 9.9668$ (3) Å
$b = 10.8210$ (3) Å
$c = 16.5299$ (5) Å
$\beta = 102.351$ (2)°
$V = 1741.50$ (9) $Å^3$
$Z = 4$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.61$ mm^{-1}
$T = 123$ (2) K
Needle, colourless
0.35 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{min} = 0.880$, $T_{max} = 0.908$
31141 measured reflections
7120 independent reflections
5777 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 27.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.067$
$S = 1.06$
7120 reflections
394 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0138P)^2 + 2.3495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.92$ e $Å^{-3}$
$\Delta\rho_{min} = -0.57$ e $Å^{-3}$
Absolute structure: Flack (1983), 3074 Friedel pairs
Flack parameter: −0.04 (2)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1[i]	2.293 (5)	Cd2—N4[iii]	2.294 (5)
Cd1—N3[ii]	2.320 (5)	Cd2—N5[iv]	2.341 (5)
Cd1—N2[ii]	2.369 (5)	Cd2—N6[iv]	2.361 (6)
Cd1—S3	2.6749 (15)	Cd2—S5	2.6925 (15)
Cd1—S1	2.7231 (15)	Cd2—S4	2.7097 (15)
Cd1—S2	2.7350 (15)	Cd2—S6	2.762 (2)
C1—S1—Cd1	94.81 (18)	C2—N2—Cd1[i]	144.8 (4)
C2—S2—Cd1	99.67 (17)	C3—N3—Cd1[i]	146.7 (4)
C3—S3—Cd1	99.07 (18)	C4—N4—Cd2[iv]	155.3 (4)
C4—S4—Cd2	95.24 (18)	C5—N5—Cd2[iii]	149.3 (4)
C5—S5—Cd2	98.12 (18)	C6—S6—Cd2	102.2 (2)
C1—N1—Cd1[ii]	155.1 (4)	C6—N6—Cd2[iii]	140.2 (6)

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

One SCN^- ligand (S6/C6/N6) was modelled as disordered by a rotation about the C atom, giving two S and two N sites. The site occupancies of the two components were refined to 0.911 (7):0.089 (7). All H atoms were placed in geometrically idealized positions and refined using a riding model: C—H = 0.95 Å for CH, 0.99 Å for CH_2 and 0.98 Å for CH_3; $U_{iso}(H) = 1.2U_{eq}(C)$ for CH and CH_2, and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3. We have noted that many crystals from the sample were twinned so that they appeared *C*-centred monoclinic.

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

RB thanks the CSIR, New Delhi, India, for providing financial support for this work.

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supporting information

Acta Cryst. (2006). E**62**, m1630–m1632   [https://doi.org/10.1107/S1600536806022938]

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β = 102.351 (2)°
V = 1741.50 (9) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.666 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 23608 reflections
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μ = 1.61 mm^{-1}
T = 123 K
Needle, colourless
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Radiation source: fine-focus sealed tube
Graphite monochromator
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7120 independent reflections
5777 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.1°, θ_{min} = 1.3°
$h = -12\rightarrow12$
$k = -13\rightarrow13$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.067
S = 1.06
7120 reflections
394 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0138P)^2 + 2.3495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: −0.04 (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}	Occ. (<1)
Cd1	0.54939 (4)	1.08483 (3)	−0.48099 (2)	0.02172 (11)	
Cd2	1.04903 (4)	0.95438 (3)	0.00501 (2)	0.02304 (12)	
S1	0.75935 (15)	0.93665 (14)	−0.40456 (10)	0.0332 (4)	
S2	0.73753 (15)	1.21949 (14)	−0.54232 (10)	0.0324 (4)	
S3	0.58885 (15)	1.21984 (14)	−0.34235 (9)	0.0289 (3)	
S4	1.24706 (14)	1.09470 (15)	−0.03894 (10)	0.0347 (4)	
S5	1.25651 (15)	0.81422 (14)	0.08814 (10)	0.0322 (4)	
N1	0.6246 (5)	0.7116 (5)	−0.4534 (3)	0.0304 (12)	
N2	0.6041 (4)	1.4486 (5)	−0.5656 (3)	0.0301 (11)	
N3	0.4838 (5)	1.4480 (5)	−0.4084 (3)	0.0308 (11)	
N4	1.1085 (5)	1.3203 (4)	−0.0389 (3)	0.0294 (11)	
N5	1.1295 (4)	0.5817 (5)	0.0633 (3)	0.0282 (10)	
N7	0.9758 (5)	1.5170 (4)	−0.3537 (3)	0.0278 (12)	
N8	1.4800 (5)	1.3837 (5)	0.1731 (3)	0.0277 (12)	
C1	0.6774 (5)	0.8053 (5)	−0.4350 (3)	0.0245 (13)	
C2	0.6582 (5)	1.3533 (5)	−0.5551 (3)	0.0205 (12)	
C3	0.5262 (5)	1.3537 (5)	−0.3828 (3)	0.0216 (12)	
C4	1.1641 (6)	1.2271 (5)	−0.0387 (3)	0.0276 (13)	
C5	1.1788 (5)	0.6776 (5)	0.0729 (3)	0.0231 (12)	
C6	0.9806 (6)	0.6968 (6)	−0.1253 (3)	0.0275 (13)	
C7	1.0872 (5)	1.4559 (6)	−0.2890 (3)	0.0269 (12)	
H7A	1.1773	1.4901	−0.2937	0.032*	
H7B	1.0724	1.4774	−0.2333	0.032*	
C8	1.0916 (5)	1.3183 (5)	−0.2964 (3)	0.0246 (12)	
C9	1.1779 (5)	1.2627 (6)	−0.3405 (4)	0.0342 (15)	
H9	1.2359	1.3122	−0.3660	0.041*	
C10	1.1805 (6)	1.1351 (6)	−0.3480 (4)	0.0431 (18)	
H10	1.2400	1.0974	−0.3786	0.052*	
C11	1.0970 (6)	1.0634 (6)	−0.3112 (4)	0.0429 (19)	
H11	1.0968	0.9761	−0.3176	0.051*	
C12	1.0144 (6)	1.1170 (6)	−0.2653 (4)	0.0394 (16)	
H12	0.9588	1.0668	−0.2386	0.047*	
C13	1.0112 (6)	1.2443 (5)	−0.2575 (4)	0.0334 (15)	
H13	0.9536	1.2810	−0.2253	0.040*	
C14	0.8361 (5)	1.4800 (5)	−0.3441 (4)	0.0417 (17)	

H14A	0.7669	1.5279	−0.3826	0.063*	
H14B	0.8272	1.4960	−0.2872	0.063*	
H14C	0.8223	1.3917	−0.3564	0.063*	
C15	0.9914 (7)	1.4849 (6)	−0.4392 (4)	0.0453 (18)	
H15A	0.9195	1.5265	−0.4798	0.068*	
H15B	0.9830	1.3953	−0.4471	0.068*	
H15C	1.0818	1.5120	−0.4466	0.068*	
C16	0.9914 (7)	1.6546 (6)	−0.3426 (4)	0.0325 (16)	
H16A	0.9700	1.6785	−0.2896	0.049*	
H16B	0.9283	1.6966	−0.3879	0.049*	
H16C	1.0861	1.6784	−0.3432	0.049*	
C17	1.6052 (5)	1.3104 (5)	0.2175 (3)	0.0304 (14)	
H17A	1.6892	1.3514	0.2078	0.036*	
H17B	1.6087	1.3125	0.2778	0.036*	
C18	1.6058 (5)	1.1769 (5)	0.1900 (3)	0.0254 (13)	
C19	1.6736 (6)	1.1449 (6)	0.1271 (4)	0.0298 (14)	
H19	1.7156	1.2072	0.1004	0.036*	
C20	1.6796 (6)	1.0236 (6)	0.1038 (4)	0.0283 (14)	
H20	1.7275	1.0022	0.0619	0.034*	
C21	1.6171 (6)	0.9331 (6)	0.1405 (3)	0.0302 (14)	
H21	1.6222	0.8495	0.1239	0.036*	
C22	1.5470 (6)	0.9625 (7)	0.2011 (3)	0.0315 (14)	
H22	1.5010	0.8999	0.2250	0.038*	
C23	1.5441 (5)	1.0826 (6)	0.2268 (3)	0.0307 (13)	
H23	1.4993	1.1021	0.2705	0.037*	
C24	1.3513 (6)	1.3350 (8)	0.1914 (5)	0.062 (2)	
H24A	1.3357	1.2507	0.1698	0.093*	
H24B	1.2743	1.3878	0.1652	0.093*	
H24C	1.3584	1.3342	0.2515	0.093*	
C25	1.4688 (7)	1.3821 (6)	0.0818 (4)	0.0435 (17)	
H25A	1.3919	1.4346	0.0550	0.065*	
H25B	1.4530	1.2973	0.0612	0.065*	
H25C	1.5542	1.4135	0.0690	0.065*	
C26	1.5050 (8)	1.5163 (6)	0.2024 (5)	0.057 (2)	
H26A	1.5179	1.5193	0.2628	0.085*	
H26B	1.4257	1.5672	0.1772	0.085*	
H26C	1.5874	1.5481	0.1861	0.085*	
S6	1.02410 (17)	0.83781 (15)	−0.14613 (13)	0.0269 (6)	0.911 (7)
N6	0.9539 (8)	0.5939 (6)	−0.1144 (4)	0.0315 (13)	0.911 (7)
S6A	0.890 (2)	0.586 (2)	−0.1443 (11)	0.020 (5)*	0.089 (7)
N6A	1.012 (6)	0.816 (6)	−0.106 (4)	0.026 (15)*	0.089 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0238 (3)	0.0129 (2)	0.0283 (2)	0.0003 (2)	0.00529 (18)	−0.00081 (19)
Cd2	0.0250 (3)	0.0116 (2)	0.0341 (2)	0.0008 (2)	0.00975 (19)	−0.00035 (19)
S1	0.0286 (8)	0.0151 (8)	0.0492 (10)	−0.0008 (7)	−0.0069 (7)	0.0002 (7)

S2	0.0312 (8)	0.0200 (8)	0.0515 (10)	0.0061 (7)	0.0211 (8)	0.0064 (7)
S3	0.0395 (8)	0.0176 (8)	0.0287 (8)	−0.0013 (7)	0.0052 (7)	0.0011 (6)
S4	0.0292 (8)	0.0170 (8)	0.0629 (10)	0.0011 (8)	0.0215 (7)	−0.0004 (8)
S5	0.0293 (8)	0.0170 (8)	0.0449 (10)	−0.0048 (7)	−0.0043 (7)	0.0013 (7)
N1	0.031 (3)	0.015 (3)	0.037 (3)	0.002 (2)	−0.010 (2)	0.004 (2)
N2	0.027 (2)	0.021 (3)	0.046 (3)	0.000 (3)	0.015 (2)	0.010 (3)
N3	0.047 (3)	0.022 (3)	0.024 (3)	0.003 (3)	0.008 (2)	0.003 (3)
N4	0.036 (3)	0.012 (3)	0.045 (3)	−0.002 (2)	0.019 (2)	0.002 (2)
N5	0.025 (2)	0.012 (2)	0.048 (3)	−0.007 (2)	0.010 (2)	−0.006 (3)
N7	0.022 (3)	0.021 (3)	0.040 (3)	−0.002 (2)	0.004 (2)	0.002 (2)
N8	0.031 (3)	0.024 (3)	0.028 (3)	0.010 (2)	0.004 (2)	−0.001 (2)
C1	0.022 (3)	0.017 (3)	0.033 (3)	0.010 (3)	0.003 (2)	0.002 (3)
C2	0.019 (3)	0.025 (3)	0.021 (3)	−0.003 (3)	0.010 (2)	0.002 (2)
C3	0.026 (3)	0.022 (3)	0.017 (3)	−0.004 (3)	0.005 (2)	−0.004 (2)
C4	0.036 (3)	0.018 (3)	0.033 (3)	−0.012 (3)	0.016 (3)	0.001 (3)
C5	0.019 (3)	0.026 (3)	0.024 (3)	0.005 (3)	0.002 (2)	−0.002 (3)
C6	0.035 (3)	0.026 (4)	0.024 (3)	0.004 (3)	0.013 (3)	0.001 (3)
C7	0.021 (3)	0.028 (3)	0.029 (3)	−0.003 (3)	0.000 (2)	−0.007 (3)
C8	0.020 (3)	0.021 (3)	0.031 (3)	0.005 (3)	0.003 (2)	−0.005 (3)
C9	0.013 (3)	0.043 (4)	0.045 (4)	0.000 (3)	0.004 (3)	−0.011 (3)
C10	0.025 (4)	0.035 (4)	0.066 (5)	0.006 (3)	0.001 (3)	−0.023 (3)
C11	0.038 (4)	0.021 (4)	0.057 (5)	0.006 (3)	−0.018 (3)	−0.008 (3)
C12	0.042 (4)	0.025 (4)	0.045 (4)	0.001 (3)	−0.004 (3)	0.009 (3)
C13	0.039 (4)	0.029 (4)	0.030 (3)	0.008 (3)	0.001 (3)	0.002 (3)
C14	0.021 (3)	0.018 (4)	0.082 (5)	0.001 (3)	0.003 (3)	0.013 (3)
C15	0.074 (5)	0.029 (4)	0.029 (4)	−0.012 (3)	0.004 (3)	−0.010 (3)
C16	0.034 (4)	0.021 (4)	0.045 (4)	0.002 (3)	0.015 (3)	0.001 (3)
C17	0.025 (3)	0.036 (4)	0.027 (3)	0.007 (3)	0.000 (3)	−0.002 (3)
C18	0.022 (3)	0.026 (3)	0.026 (3)	0.000 (3)	0.000 (3)	−0.004 (3)
C19	0.025 (3)	0.033 (4)	0.032 (4)	−0.006 (3)	0.008 (3)	−0.001 (3)
C20	0.024 (3)	0.035 (4)	0.026 (3)	−0.002 (3)	0.008 (3)	−0.006 (3)
C21	0.037 (4)	0.020 (4)	0.030 (3)	0.001 (3)	−0.002 (3)	−0.004 (3)
C22	0.035 (4)	0.028 (4)	0.030 (3)	−0.007 (3)	0.004 (3)	0.001 (3)
C23	0.028 (3)	0.039 (4)	0.024 (3)	0.007 (3)	0.004 (2)	0.002 (3)
C24	0.032 (4)	0.070 (5)	0.092 (6)	0.015 (4)	0.033 (4)	0.018 (5)
C25	0.057 (4)	0.034 (4)	0.034 (4)	0.004 (3)	−0.002 (3)	0.003 (3)
C26	0.063 (5)	0.035 (4)	0.061 (5)	0.024 (4)	−0.010 (4)	−0.015 (4)
S6	0.0374 (10)	0.0153 (9)	0.0305 (13)	0.0010 (8)	0.0127 (8)	0.0029 (7)
N6	0.035 (4)	0.020 (3)	0.039 (3)	0.001 (3)	0.007 (3)	0.004 (3)

Geometric parameters (Å, º)

Cd1—N1^{i}	2.293 (5)	C8—C13	1.385 (8)
Cd1—N3^{ii}	2.320 (5)	C9—C10	1.387 (8)
Cd1—N2^{ii}	2.369 (5)	C9—H9	0.950
Cd1—S3	2.6749 (15)	C10—C11	1.373 (9)
Cd1—S1	2.7231 (15)	C10—H10	0.950
Cd1—S2	2.7350 (15)	C11—C12	1.362 (9)

Cd2—N4^{iii}	2.294 (5)	C11—H11	0.950
Cd2—N6A	2.34 (6)	C12—C13	1.385 (8)
Cd2—N5^{iv}	2.341 (5)	C12—H12	0.950
Cd2—N6^{iv}	2.361 (6)	C13—H13	0.950
Cd2—S6A^{iv}	2.664 (19)	C14—H14A	0.980
Cd2—S5	2.6925 (15)	C14—H14B	0.980
Cd2—S4	2.7097 (15)	C14—H14C	0.980
Cd2—S6	2.762 (2)	C15—H15A	0.980
S1—C1	1.663 (6)	C15—H15B	0.980
S2—C2	1.642 (6)	C15—H15C	0.980
S3—C3	1.661 (6)	C16—H16A	0.980
S4—C4	1.654 (6)	C16—H16B	0.980
S5—C5	1.663 (6)	C16—H16C	0.980
N1—C1	1.152 (7)	C17—C18	1.514 (8)
N1—Cd1^{ii}	2.293 (5)	C17—H17A	0.990
N2—C2	1.159 (7)	C17—H17B	0.990
N2—Cd1^{i}	2.369 (5)	C18—C23	1.396 (8)
N3—C3	1.150 (7)	C18—C19	1.400 (7)
N3—Cd1^{i}	2.320 (5)	C19—C20	1.373 (7)
N4—C4	1.150 (7)	C19—H19	0.950
N4—Cd2^{iv}	2.294 (5)	C20—C21	1.369 (8)
N5—C5	1.145 (7)	C20—H20	0.950
N5—Cd2^{iii}	2.341 (5)	C21—C22	1.377 (7)
N7—C14	1.490 (7)	C21—H21	0.950
N7—C15	1.495 (7)	C22—C23	1.370 (9)
N7—C16	1.504 (7)	C22—H22	0.950
N7—C7	1.517 (7)	C23—H23	0.950
N8—C24	1.478 (8)	C24—H24A	0.980
N8—C25	1.489 (7)	C24—H24B	0.980
N8—C26	1.518 (8)	C24—H24C	0.980
N8—C17	1.527 (7)	C25—H25A	0.980
C6—N6	1.168 (8)	C25—H25B	0.980
C6—N6A	1.35 (6)	C25—H25C	0.980
C6—S6A	1.50 (2)	C26—H26A	0.980
C6—S6	1.642 (6)	C26—H26B	0.980
C7—C8	1.496 (8)	C26—H26C	0.980
C7—H7A	0.990	N6—Cd2^{iii}	2.361 (6)
C7—H7B	0.990	S6A—Cd2^{iii}	2.664 (19)
C8—C9	1.379 (7)		

N1^{i}—Cd1—N3^{ii}	92.47 (17)	C13—C8—C7	120.5 (5)
N1^{i}—Cd1—N2^{ii}	92.87 (17)	C8—C9—C10	120.5 (6)
N3^{ii}—Cd1—N2^{ii}	82.29 (16)	C8—C9—H9	119.8
N1^{i}—Cd1—S3	92.07 (12)	C10—C9—H9	119.8
N3^{ii}—Cd1—S3	173.44 (13)	C11—C10—C9	119.9 (6)
N2^{ii}—Cd1—S3	92.76 (12)	C11—C10—H10	120.1
N1^{i}—Cd1—S1	178.92 (13)	C9—C10—H10	120.1
N3^{ii}—Cd1—S1	87.47 (13)	C12—C11—C10	120.2 (6)

$N2^{ii}$—Cd1—S1	88.19 (12)	C12—C11—H11	119.9
S3—Cd1—S1	88.08 (5)	C10—C11—H11	119.9
$N1^{i}$—Cd1—S2	90.88 (13)	C11—C12—C13	120.3 (6)
$N3^{ii}$—Cd1—S2	92.38 (12)	C11—C12—H12	119.9
$N2^{ii}$—Cd1—S2	173.60 (12)	C13—C12—H12	119.9
S3—Cd1—S2	92.28 (5)	C12—C13—C8	120.3 (6)
S1—Cd1—S2	88.05 (5)	C12—C13—H13	119.8
$N4^{iii}$—Cd2—N6A	77.7 (18)	C8—C13—H13	119.8
$N4^{iii}$—Cd2—$N5^{iv}$	90.04 (16)	N7—C14—H14A	109.5
N6A—Cd2—$N5^{iv}$	91.2 (15)	N7—C14—H14B	109.5
$N4^{iii}$—Cd2—$N6^{iv}$	95.52 (18)	H14A—C14—H14B	109.5
N6A—Cd2—$N6^{iv}$	170.4 (14)	N7—C14—H14C	109.5
$N5^{iv}$—Cd2—$N6^{iv}$	82.0 (2)	H14A—C14—H14C	109.5
$N4^{iii}$—Cd2—$S6A^{iv}$	99.7 (4)	H14B—C14—H14C	109.5
N6A—Cd2—$S6A^{iv}$	171.9 (17)	N7—C15—H15A	109.5
$N5^{iv}$—Cd2—$S6A^{iv}$	96.5 (5)	N7—C15—H15B	109.5
$N4^{iii}$—Cd2—S5	90.59 (12)	H15A—C15—H15B	109.5
N6A—Cd2—S5	90.9 (15)	N7—C15—H15C	109.5
$N5^{iv}$—Cd2—S5	177.87 (13)	H15A—C15—H15C	109.5
$N6^{iv}$—Cd2—S5	95.9 (2)	H15B—C15—H15C	109.5
$S6A^{iv}$—Cd2—S5	81.4 (5)	N7—C16—H16A	109.5
$N4^{iii}$—Cd2—S4	174.82 (12)	N7—C16—H16B	109.5
N6A—Cd2—S4	98.5 (17)	H16A—C16—H16B	109.5
$N5^{iv}$—Cd2—S4	93.60 (12)	N7—C16—H16C	109.5
$N6^{iv}$—Cd2—S4	88.64 (15)	H16A—C16—H16C	109.5
$S6A^{iv}$—Cd2—S4	83.5 (4)	H16B—C16—H16C	109.5
S5—Cd2—S4	85.90 (5)	C18—C17—N8	114.0 (4)
$N4^{iii}$—Cd2—S6	89.88 (12)	C18—C17—H17A	108.8
N6A—Cd2—S6	13.5 (18)	N8—C17—H17A	108.8
$N5^{iv}$—Cd2—S6	85.43 (12)	C18—C17—H17B	108.8
$N6^{iv}$—Cd2—S6	166.3 (2)	N8—C17—H17B	108.8
$S6A^{iv}$—Cd2—S6	170.2 (4)	H17A—C17—H17B	107.7
S5—Cd2—S6	96.61 (5)	C23—C18—C19	118.1 (5)
S4—Cd2—S6	86.74 (5)	C23—C18—C17	122.4 (5)
C1—S1—Cd1	94.81 (18)	C19—C18—C17	119.5 (5)
C2—S2—Cd1	99.67 (17)	C20—C19—C18	120.1 (5)
C3—S3—Cd1	99.07 (18)	C20—C19—H19	119.9
C4—S4—Cd2	95.24 (18)	C18—C19—H19	119.9
C5—S5—Cd2	98.12 (18)	C21—C20—C19	120.6 (5)
C1—N1—$Cd1^{ii}$	155.1 (4)	C21—C20—H20	119.7
C2—N2—$Cd1^{i}$	144.8 (4)	C19—C20—H20	119.7
C3—N3—$Cd1^{i}$	146.7 (4)	C20—C21—C22	120.5 (6)
C4—N4—$Cd2^{iv}$	155.3 (4)	C20—C21—H21	119.8
C5—N5—$Cd2^{iii}$	149.3 (4)	C22—C21—H21	119.8
C14—N7—C15	109.0 (5)	C23—C22—C21	119.5 (6)
C14—N7—C16	109.2 (5)	C23—C22—H22	120.2
C15—N7—C16	108.4 (5)	C21—C22—H22	120.2
C14—N7—C7	111.6 (4)	C22—C23—C18	121.2 (5)

C15—N7—C7	110.9 (4)	C22—C23—H23	119.4
C16—N7—C7	107.7 (5)	C18—C23—H23	119.4
C24—N8—C25	108.9 (5)	N8—C24—H24A	109.5
C24—N8—C26	111.2 (6)	N8—C24—H24B	109.5
C25—N8—C26	107.8 (5)	H24A—C24—H24B	109.5
C24—N8—C17	111.8 (5)	N8—C24—H24C	109.5
C25—N8—C17	111.0 (5)	H24A—C24—H24C	109.5
C26—N8—C17	106.0 (5)	H24B—C24—H24C	109.5
N1—C1—S1	177.0 (5)	N8—C25—H25A	109.5
N2—C2—S2	178.2 (5)	N8—C25—H25B	109.5
N3—C3—S3	177.9 (5)	H25A—C25—H25B	109.5
N4—C4—S4	178.7 (5)	N8—C25—H25C	109.5
N5—C5—S5	177.7 (5)	H25A—C25—H25C	109.5
N6—C6—N6A	158 (3)	H25B—C25—H25C	109.5
N6A—C6—S6A	156 (3)	N8—C26—H26A	109.5
N6—C6—S6	175.6 (5)	N8—C26—H26B	109.5
S6A—C6—S6	151.2 (8)	H26A—C26—H26B	109.5
C8—C7—N7	114.0 (4)	N8—C26—H26C	109.5
C8—C7—H7A	108.8	H26A—C26—H26C	109.5
N7—C7—H7A	108.8	H26B—C26—H26C	109.5
C8—C7—H7B	108.8	C6—S6—Cd2	102.2 (2)
N7—C7—H7B	108.8	C6—N6—Cd2^{iii}	140.2 (6)
H7A—C7—H7B	107.7	C6—S6A—Cd2^{iii}	103.4 (10)
C9—C8—C13	118.8 (5)	C6—N6A—Cd2	142 (5)
C9—C8—C7	120.7 (5)		

N3^{ii}—Cd1—S1—C1	−40.4 (2)	C7—C8—C9—C10	−179.2 (5)
N2^{ii}—Cd1—S1—C1	42.0 (2)	C8—C9—C10—C11	−0.1 (10)
S3—Cd1—S1—C1	134.8 (2)	C9—C10—C11—C12	−1.9 (9)
S2—Cd1—S1—C1	−132.8 (2)	C10—C11—C12—C13	1.8 (9)
N1^{i}—Cd1—S2—C2	26.0 (2)	C11—C12—C13—C8	0.2 (9)
N3^{ii}—Cd1—S2—C2	118.5 (2)	C9—C8—C13—C12	−2.1 (8)
S3—Cd1—S2—C2	−66.1 (2)	C7—C8—C13—C12	179.2 (5)
S1—Cd1—S2—C2	−154.1 (2)	C24—N8—C17—C18	64.1 (7)
N1^{i}—Cd1—S3—C3	−24.4 (2)	C25—N8—C17—C18	−57.7 (6)
N2^{ii}—Cd1—S3—C3	−117.4 (2)	C26—N8—C17—C18	−174.6 (6)
N5^{iv}—Cd2—S4—C4	32.0 (2)	N8—C17—C18—C23	−88.5 (6)
N6^{iv}—Cd2—S4—C4	−49.9 (3)	N8—C17—C18—C19	93.3 (6)
S6A^{iv}—Cd2—S4—C4	−64.1 (5)	C23—C18—C19—C20	−0.8 (8)
S5—Cd2—S4—C4	−145.9 (2)	C17—C18—C19—C20	177.4 (5)
S6—Cd2—S4—C4	117.2 (2)	C18—C19—C20—C21	1.4 (9)
N4^{iii}—Cd2—S5—C5	31.1 (2)	C19—C20—C21—C22	0.1 (9)
N6A—Cd2—S5—C5	−46.6 (18)	C20—C21—C22—C23	−2.3 (8)
N6^{iv}—Cd2—S5—C5	126.7 (2)	C21—C22—C23—C18	2.9 (8)
S6A^{iv}—Cd2—S5—C5	130.8 (4)	C19—C18—C23—C22	−1.4 (8)
C14—N7—C7—C8	64.7 (6)	C17—C18—C23—C22	−179.5 (5)
C15—N7—C7—C8	−57.1 (6)	N4^{iii}—Cd2—S6—C6	−27.9 (2)
C16—N7—C7—C8	−175.6 (5)	N5^{iv}—Cd2—S6—C6	−118.0 (2)

N7—C7—C8—C9	94.0 (6)	N6^{iv}—Cd2—S6—C6	−141.3 (7)
N7—C7—C8—C13	−87.4 (6)	S5—Cd2—S6—C6	62.6 (2)
C13—C8—C9—C10	2.1 (8)	S4—Cd2—S6—C6	148.1 (2)

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