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Bis[*N*-(2-hydroxyethyl)-*N*-propyldithiocarbamato-$\kappa^2 S,S'$]bis(4-{[(pyridin-4-ylmethylidene)hydrazinylidene]methyl}pyridine-κN^1)cadmium

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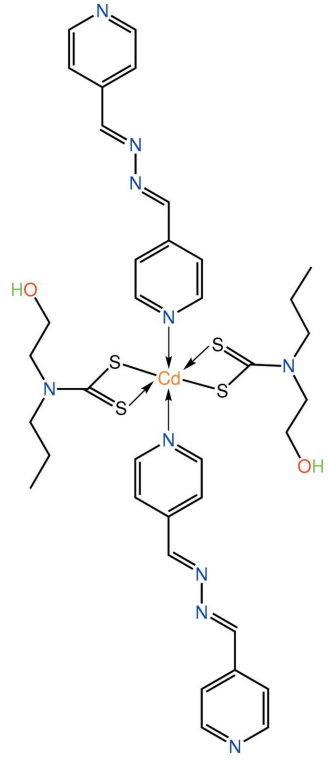
Key indicators: single-crystal X-ray study; T = 98 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.062; data-to-parameter ratio = 16.9.

The complete molecule of the title compound, $[Cd(C_6H_{12}NOS_2)_2(C_{12}H_{10}N_4)_2]$, is generated by crystallographic inversion symmetry. The distorted octahedral *trans*-N_2S_4 donor set for the Cd^{2+} ion is defined by two symmetrically *S*,*S*′-chelating dithiocarbamate anions and two pyridine N atoms derived from two monodentate 4-pyridinealdazine (or 4-{[(pyridin-4-ylmethylidene)hydrazinylidene}methyl]pyridine) molecules [dihedral angle between the aromatic rings = 17.33 (8)°]. In the crystal, molecules are connected into a supramolecular chain *via* O—H···N hydrogen bonds involving the 4-pyridinealdazine N atoms not involved in coordination to cadmium. Weak C—H···O and C—H···N links consolidate the packing.

Related literature

For background to supramolecular coordination polymers of zinc-triad 1,1-dithiolates, see: Tiekink (2003). For the use of steric effects to control supramolecular aggregation patterns, see: Chen *et al.* (2006). For structural studies on hydroxyl-substituted dithiocarbamate ligands, see Benson *et al.* (2007); Song & Tiekink (2009).



Experimental

Crystal data

$[Cd(C_6H_{12}NOS_2)_2(C_{12}H_{10}N_4)_2]$
M_r = 889.45
Triclinic, $P\overline{1}$
a = 8.532 (3) Å
b = 10.951 (4) Å
c = 11.184 (5) Å
α = 79.59 (3)°
β = 88.06 (3)°
γ = 78.23 (2)°
V = 1006.2 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 98 K
0.25 × 0.16 × 0.04 mm

Data collection

Rigaku AFC12/SATURN724 CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.719, T_{max} = 1
10677 measured reflections
4150 independent reflections
4009 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.062
S = 1.08
4150 reflections
245 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—S1	2.6379 (10)	Cd—N2	2.5403 (17)
Cd—S2	2.6626 (10)		
S1—Cd—S2	68.83 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*o*···N5^{i}	0.84 (2)	1.98 (2)	2.810 (2)	176 (2)
C10—H10···O1^{ii}	0.95	2.55	3.480 (3)	168
C3—H3a···N4^{iii}	0.99	2.61	3.369 (3)	134

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

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: PATTY in *DIRDIF* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5795).

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supplementary materials

Acta Cryst. (2011). E**67**, m320-m321 [**doi:10.1107/S1600536811004508**]

Bis[*N*-(2-hydroxyethyl)-*N*-propyldithiocarbamato-$\kappa^2 S,S'$]bis(4-{[(pyridin-4-ylmethylidene)hydrazinylidene]methyl}pyridine-κN^1)cadmium

G. A. Broker and E. R. T. Tiekink

Comment

Interest in the title compound, (I), relates to controlling supramolecular aggregation patterns in the zinc-triad 1,1-thiolates (Tiekink, 2003; Chen *et al.*, 2006). With functionalized dithiocarbamate ligands carrying hydrogen bonding potential, smaller aggregates can be linked into 2-D and 3-D architectures (Benson *et al.*, 2007; Song & Tiekink, 2009). In (I), the cadmium atom is located on a centre of inversion and is chelated by symmetrically coordinating dithiocarbamate ligands, Table 1 and Fig. 1. The octahedral N_2S_4 donor set is completed by two pyridine-N atoms derived from two monodentate 4-pyridinealdazine ligands.

The monomeric molecules are connected into a supramolecular chain *via* O–H···N hydrogen bonds, Table 2, that lead to the formation of 40-membered $[CdSCNC_2OH\cdots NC_4N_2C_4N]_2$ synthons, Fig. 2. These chains are linked into layers *via* C–H···O interactions, Table 1, which that stack along [1 0 1]; consolidation of these layers into a 3-D array is afforded by C—H···N_{azo} contacts, Table 2 and Fig. 3.

Experimental

Compound (I) was prepared following the standard literature procedure (Song & Tiekink, 2009) from the reaction of $Cd[S_2CN(CH_2CH_2OH)(nPr)]_2$ and 4-[(1*E*)-[(*E*)-2-(pyridin-4-ylmethylidene)hydrazin-1-ylidene]methyl]pyridine (Sigma Aldrich). Yellow plates of (I) were obtained from the slow evaporation of a chloroform/acetonitrile (3/1) solution.

Refinement

C-bound H-atoms were placed in calculated positions (C–H 0.95–0.99 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2–1.5U_{eq}(C). The O-bound H-atom was located in a difference Fourier map and refined with an O–H restraint of 0.84±0.01 Å, and with U_{iso}(H) = 1.5U_{eq}(O). The reflection ($\bar{8}$ $\bar{1}$ 2) was removed from the final refinement owing to poor agreement.

Figures

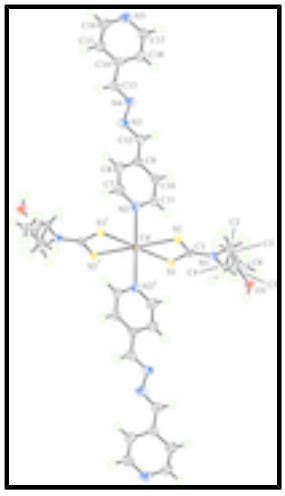

Fig. 1. Molecular structure of (I) showing displacement ellipsoids at the 70% probability level. The Cd atom is located on a centre of inversion and *i* = 1 - *x*, 1 - *y*, 1 - *z*.

Fig. 2. Supramolecular chain in (I) mediated by O–H···N (orange dashed lines) hydrogen bonds. Colour code: Cd, orange; S, yellow; O, red; N, blue; C, grey; and H, green.

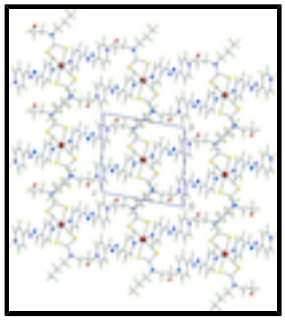

Fig. 3. Unit-cell contents in (I) viewed in projection down the *a* axis.

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Crystal data

$[Cd(C_6H_{12}NOS_2)_2(C_{12}H_{10}N_4)_2]$	$Z = 1$
$M_r = 889.45$	$F(000) = 458$
Triclinic, $P\overline{1}$	$D_x = 1.468$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
$a = 8.532$ (3) Å	Cell parameters from 3485 reflections
$b = 10.951$ (4) Å	$\theta = 2.4$–$30.3°$
$c = 11.184$ (5) Å	$\mu = 0.80$ mm^{-1}
$\alpha = 79.59$ (3)°	$T = 98$ K
$\beta = 88.06$ (3)°	Plate, yellow
$\gamma = 78.23$ (2)°	0.25 × 0.16 × 0.04 mm
$V = 1006.2$ (7) Å^3	

Data collection

Rigaku AFC12K/SATURN724 CCD diffractometer	4150 independent reflections
Radiation source: fine-focus sealed tube	4009 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
ω scans	$\theta_{max} = 26.5°$, $\theta_{min} = 2.4°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -10 \rightarrow 10$
$T_{min} = 0.719$, $T_{max} = 1$	$k = -13 \rightarrow 12$
10677 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.025$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.062$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.08$	$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.6008P]$ where $P = (F_o^2 + 2F_c^2)/3$
4150 reflections	$(\Delta/\sigma)_{max} < 0.001$
245 parameters	$\Delta\rho_{max} = 0.40$ e Å^{-3}
1 restraint	$\Delta\rho_{min} = -0.40$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
Cd	0.5000	0.5000	0.5000	0.01706 (6)
S1	0.67567 (5)	0.26992 (4)	0.55937 (3)	0.01562 (9)
S2	0.48740 (5)	0.36286 (4)	0.32801 (4)	0.01587 (9)
O1	0.88422 (15)	0.05660 (12)	0.17754 (11)	0.0223 (3)
H1o	0.954 (2)	0.094 (2)	0.1432 (19)	0.033*
N1	0.67484 (15)	0.13324 (12)	0.38469 (11)	0.0120 (3)

N2	0.26143 (17)	0.42763 (14)	0.61140 (13)	0.0192 (3)
N3	−0.25800 (17)	0.36129 (14)	0.82625 (13)	0.0194 (3)
N4	−0.37162 (17)	0.28924 (14)	0.87834 (12)	0.0191 (3)
N5	−0.88990 (18)	0.19365 (15)	1.06431 (14)	0.0245 (3)
C1	0.61822 (18)	0.24449 (15)	0.41986 (14)	0.0135 (3)
C2	0.62455 (19)	0.10536 (15)	0.26935 (14)	0.0156 (3)
H2A	0.5139	0.1526	0.2501	0.019*
H2B	0.6239	0.0138	0.2796	0.019*
C3	0.7325 (2)	0.14035 (16)	0.16368 (15)	0.0196 (3)
H3A	0.6824	0.1356	0.0866	0.024*
H3B	0.7465	0.2285	0.1601	0.024*
C4	0.79259 (19)	0.03218 (15)	0.45840 (14)	0.0150 (3)
H4A	0.8604	0.0717	0.5037	0.018*
H4B	0.8630	−0.0158	0.4033	0.018*
C5	0.7154 (2)	−0.05962 (16)	0.54826 (15)	0.0185 (3)
H5A	0.6421	−0.0957	0.5043	0.022*
H5B	0.6517	−0.0137	0.6080	0.022*
C6	0.8430 (2)	−0.16666 (17)	0.61485 (17)	0.0239 (4)
H6A	0.7911	−0.2254	0.6715	0.036*
H6B	0.9137	−0.1311	0.6602	0.036*
H6C	0.9059	−0.2121	0.5557	0.036*
C7	0.1257 (2)	0.50814 (17)	0.63223 (18)	0.0254 (4)
H7	0.1197	0.5963	0.6049	0.031*
C8	−0.0057 (2)	0.46933 (17)	0.69130 (17)	0.0238 (4)
H8	−0.0989	0.5297	0.7041	0.029*
C9	0.0008 (2)	0.34018 (16)	0.73174 (14)	0.0169 (3)
C10	0.1403 (2)	0.25663 (16)	0.70970 (16)	0.0203 (3)
H10	0.1493	0.1679	0.7352	0.024*
C11	0.2661 (2)	0.30418 (16)	0.65018 (16)	0.0205 (3)
H11	0.3608	0.2458	0.6362	0.025*
C12	−0.1326 (2)	0.28869 (16)	0.79403 (14)	0.0177 (3)
H12	−0.1255	0.1995	0.8107	0.021*
C13	−0.5012 (2)	0.35972 (17)	0.90688 (15)	0.0200 (3)
H13	−0.5119	0.4492	0.8929	0.024*
C14	−0.6338 (2)	0.30118 (17)	0.96168 (14)	0.0188 (3)
C15	−0.7640 (2)	0.37321 (18)	1.01209 (17)	0.0248 (4)
H15	−0.7681	0.4604	1.0127	0.030*
C16	−0.8877 (2)	0.31554 (19)	1.06143 (17)	0.0269 (4)
H16	−0.9762	0.3659	1.0952	0.032*
C17	−0.7628 (2)	0.12403 (18)	1.01712 (16)	0.0247 (4)
H17	−0.7612	0.0367	1.0192	0.030*
C18	−0.6341 (2)	0.17338 (18)	0.96559 (16)	0.0228 (4)
H18	−0.5468	0.1206	0.9332	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.01757 (10)	0.01303 (10)	0.02083 (10)	−0.00255 (7)	0.00354 (7)	−0.00493 (7)

S1	0.0170 (2)	0.01481 (19)	0.01487 (19)	−0.00153 (15)	−0.00065 (15)	−0.00389 (15)
S2	0.0170 (2)	0.01234 (19)	0.0169 (2)	−0.00014 (15)	−0.00203 (15)	−0.00179 (15)
O1	0.0183 (6)	0.0224 (6)	0.0251 (6)	−0.0043 (5)	0.0080 (5)	−0.0026 (5)
N1	0.0114 (6)	0.0119 (6)	0.0122 (6)	−0.0014 (5)	−0.0004 (5)	−0.0016 (5)
N2	0.0185 (7)	0.0181 (7)	0.0218 (7)	−0.0050 (6)	0.0034 (6)	−0.0048 (6)
N3	0.0178 (7)	0.0218 (7)	0.0184 (7)	−0.0064 (6)	0.0024 (5)	−0.0007 (6)
N4	0.0188 (7)	0.0228 (7)	0.0161 (7)	−0.0080 (6)	0.0024 (5)	−0.0003 (6)
N5	0.0222 (8)	0.0305 (9)	0.0219 (8)	−0.0094 (7)	0.0047 (6)	−0.0035 (6)
C1	0.0114 (7)	0.0144 (8)	0.0147 (7)	−0.0042 (6)	0.0032 (6)	−0.0014 (6)
C2	0.0165 (8)	0.0145 (8)	0.0158 (8)	−0.0018 (6)	0.0002 (6)	−0.0037 (6)
C3	0.0222 (9)	0.0195 (8)	0.0156 (8)	−0.0012 (7)	0.0027 (6)	−0.0030 (6)
C4	0.0127 (7)	0.0138 (8)	0.0169 (8)	0.0004 (6)	−0.0007 (6)	−0.0020 (6)
C5	0.0167 (8)	0.0168 (8)	0.0210 (8)	−0.0043 (7)	0.0009 (6)	−0.0003 (6)
C6	0.0224 (9)	0.0202 (9)	0.0266 (9)	−0.0051 (7)	−0.0034 (7)	0.0044 (7)
C7	0.0230 (9)	0.0162 (8)	0.0348 (10)	−0.0033 (7)	0.0087 (8)	−0.0008 (7)
C8	0.0174 (9)	0.0198 (9)	0.0320 (10)	−0.0012 (7)	0.0055 (7)	−0.0023 (7)
C9	0.0168 (8)	0.0207 (8)	0.0146 (8)	−0.0062 (7)	0.0003 (6)	−0.0039 (6)
C10	0.0217 (9)	0.0158 (8)	0.0245 (9)	−0.0048 (7)	0.0021 (7)	−0.0055 (7)
C11	0.0193 (8)	0.0175 (8)	0.0259 (9)	−0.0031 (7)	0.0036 (7)	−0.0083 (7)
C12	0.0181 (8)	0.0198 (8)	0.0153 (8)	−0.0055 (7)	−0.0024 (6)	−0.0015 (6)
C13	0.0198 (9)	0.0213 (9)	0.0178 (8)	−0.0049 (7)	0.0006 (6)	0.0003 (7)
C14	0.0171 (8)	0.0241 (9)	0.0146 (8)	−0.0054 (7)	0.0000 (6)	−0.0003 (6)
C15	0.0238 (9)	0.0215 (9)	0.0283 (9)	−0.0043 (7)	0.0040 (7)	−0.0039 (7)
C16	0.0206 (9)	0.0304 (10)	0.0290 (10)	−0.0037 (8)	0.0076 (7)	−0.0062 (8)
C17	0.0255 (9)	0.0246 (9)	0.0260 (9)	−0.0096 (8)	0.0052 (7)	−0.0056 (7)
C18	0.0216 (9)	0.0248 (9)	0.0229 (9)	−0.0054 (7)	0.0045 (7)	−0.0067 (7)

Geometric parameters (Å, °)

Cd—S1	2.6379 (10)	C4—H4B	0.9900
Cd—S2	2.6626 (10)	C5—C6	1.527 (2)
Cd—N2	2.5403 (17)	C5—H5A	0.9900
Cd—S1^{i}	2.6379 (10)	C5—H5B	0.9900
Cd—S2^{i}	2.6626 (10)	C6—H6A	0.9800
Cd—N2^{i}	2.5403 (17)	C6—H6B	0.9800
S1—C1	1.7369 (17)	C6—H6C	0.9800
S2—C1	1.7286 (18)	C7—C8	1.385 (2)
O1—C3	1.421 (2)	C7—H7	0.9500
O1—H1o	0.835 (10)	C8—C9	1.395 (2)
N1—C1	1.339 (2)	C8—H8	0.9500
N1—C2	1.475 (2)	C9—C10	1.390 (2)
N1—C4	1.479 (2)	C9—C12	1.471 (2)
N2—C11	1.336 (2)	C10—C11	1.386 (2)
N2—C7	1.347 (2)	C10—H10	0.9500
N3—C12	1.280 (2)	C11—H11	0.9500
N3—N4	1.418 (2)	C12—H12	0.9500
N4—C13	1.279 (2)	C13—C14	1.475 (2)
N5—C16	1.333 (3)	C13—H13	0.9500

N5—C17	1.344 (2)	C14—C15	1.391 (2)
C2—C3	1.516 (2)	C14—C18	1.393 (3)
C2—H2A	0.9900	C15—C16	1.388 (3)
C2—H2B	0.9900	C15—H15	0.9500
C3—H3A	0.9900	C16—H16	0.9500
C3—H3B	0.9900	C17—C18	1.385 (2)
C4—C5	1.521 (2)	C17—H17	0.9500
C4—H4A	0.9900	C18—H18	0.9500
$N2^{i}$—Cd—N2	180	C4—C5—C6	110.58 (14)
$N2^{i}$—Cd—S1	89.42 (4)	C4—C5—H5A	109.5
N2—Cd—S1	90.58 (4)	C6—C5—H5A	109.5
$N2^{i}$—Cd—$S1^{i}$	90.58 (4)	C4—C5—H5B	109.5
N2—Cd—$S1^{i}$	89.42 (4)	C6—C5—H5B	109.5
S1—Cd—$S1^{i}$	180	H5A—C5—H5B	108.1
$N2^{i}$—Cd—S2	87.62 (4)	C5—C6—H6A	109.5
N2—Cd—S2	92.38 (4)	C5—C6—H6B	109.5
S1—Cd—S2	68.83 (3)	H6A—C6—H6B	109.5
$S1^{i}$—Cd—S2	111.17 (3)	C5—C6—H6C	109.5
$N2^{i}$—Cd—$S2^{i}$	92.38 (4)	H6A—C6—H6C	109.5
N2—Cd—$S2^{i}$	87.62 (4)	H6B—C6—H6C	109.5
S1—Cd—$S2^{i}$	111.17 (3)	N2—C7—C8	123.52 (17)
$S1^{i}$—Cd—$S2^{i}$	68.83 (3)	N2—C7—H7	118.2
S2—Cd—$S2^{i}$	180	C8—C7—H7	118.2
C1—S1—Cd	86.05 (6)	C7—C8—C9	119.02 (16)
C1—S2—Cd	85.43 (6)	C7—C8—H8	120.5
C3—O1—H1o	109.5 (16)	C9—C8—H8	120.5
C1—N1—C2	121.74 (13)	C10—C9—C8	117.67 (15)
C1—N1—C4	121.96 (13)	C10—C9—C12	118.88 (15)
C2—N1—C4	116.29 (13)	C8—C9—C12	123.44 (16)
C11—N2—C7	116.95 (15)	C11—C10—C9	119.30 (16)
C11—N2—Cd	119.88 (11)	C11—C10—H10	120.3
C7—N2—Cd	123.16 (11)	C9—C10—H10	120.3
C12—N3—N4	110.47 (14)	N2—C11—C10	123.54 (16)
C13—N4—N3	111.93 (14)	N2—C11—H11	118.2
C16—N5—C17	116.98 (16)	C10—C11—H11	118.2
N1—C1—S2	120.59 (12)	N3—C12—C9	121.48 (16)
N1—C1—S1	119.77 (12)	N3—C12—H12	119.3
S2—C1—S1	119.64 (10)	C9—C12—H12	119.3
N1—C2—C3	113.01 (13)	N4—C13—C14	119.59 (16)
N1—C2—H2A	109.0	N4—C13—H13	120.2
C3—C2—H2A	109.0	C14—C13—H13	120.2
N1—C2—H2B	109.0	C15—C14—C18	117.63 (16)
C3—C2—H2B	109.0	C15—C14—C13	120.38 (16)
H2A—C2—H2B	107.8	C18—C14—C13	121.99 (16)
O1—C3—C2	110.27 (14)	C16—C15—C14	118.89 (17)
O1—C3—H3A	109.6	C16—C15—H15	120.6

C2—C3—H3A	109.6	C14—C15—H15	120.6
O1—C3—H3B	109.6	N5—C16—C15	123.90 (17)
C2—C3—H3B	109.6	N5—C16—H16	118.0
H3A—C3—H3B	108.1	C15—C16—H16	118.0
N1—C4—C5	113.22 (13)	N5—C17—C18	123.21 (17)
N1—C4—H4A	108.9	N5—C17—H17	118.4
C5—C4—H4A	108.9	C18—C17—H17	118.4
N1—C4—H4B	108.9	C17—C18—C14	119.38 (17)
C5—C4—H4B	108.9	C17—C18—H18	120.3
H4A—C4—H4B	107.7	C14—C18—H18	120.3
$N2^{i}$—Cd—S1—C1	−86.27 (7)	C4—N1—C2—C3	−87.99 (17)
N2—Cd—S1—C1	93.73 (7)	N1—C2—C3—O1	70.19 (17)
$S1^{i}$—Cd—S1—C1	95 (100)	C1—N1—C4—C5	90.95 (18)
S2—Cd—S1—C1	1.40 (5)	C2—N1—C4—C5	−89.78 (16)
$S2^{i}$—Cd—S1—C1	−178.60 (5)	N1—C4—C5—C6	175.96 (13)
$N2^{i}$—Cd—S2—C1	88.89 (7)	C11—N2—C7—C8	0.3 (3)
N2—Cd—S2—C1	−91.11 (7)	Cd—N2—C7—C8	179.02 (14)
S1—Cd—S2—C1	−1.41 (5)	N2—C7—C8—C9	−0.1 (3)
$S1^{i}$—Cd—S2—C1	178.59 (5)	C7—C8—C9—C10	−0.3 (3)
$S2^{i}$—Cd—S2—C1	−29 (100)	C7—C8—C9—C12	−179.20 (17)
$N2^{i}$—Cd—N2—C11	−146 (100)	C8—C9—C10—C11	0.5 (2)
S1—Cd—N2—C11	−10.78 (13)	C12—C9—C10—C11	179.47 (15)
$S1^{i}$—Cd—N2—C11	169.22 (13)	C7—N2—C11—C10	−0.1 (3)
S2—Cd—N2—C11	58.06 (13)	Cd—N2—C11—C10	−178.83 (13)
$S2^{i}$—Cd—N2—C11	−121.94 (13)	C9—C10—C11—N2	−0.3 (3)
$N2^{i}$—Cd—N2—C7	35 (100)	N4—N3—C12—C9	176.90 (14)
S1—Cd—N2—C7	170.58 (14)	C10—C9—C12—N3	173.70 (15)
$S1^{i}$—Cd—N2—C7	−9.42 (14)	C8—C9—C12—N3	−7.4 (3)
S2—Cd—N2—C7	−120.58 (14)	N3—N4—C13—C14	179.61 (14)
$S2^{i}$—Cd—N2—C7	59.42 (14)	N4—C13—C14—C15	169.03 (16)
C12—N3—N4—C13	−177.28 (14)	N4—C13—C14—C18	−10.7 (3)
C2—N1—C1—S2	−2.1 (2)	C18—C14—C15—C16	−1.1 (3)
C4—N1—C1—S2	177.14 (10)	C13—C14—C15—C16	179.14 (16)
C2—N1—C1—S1	177.52 (10)	C17—N5—C16—C15	0.6 (3)
C4—N1—C1—S1	−3.2 (2)	C14—C15—C16—N5	0.4 (3)
Cd—S2—C1—N1	−178.09 (12)	C16—N5—C17—C18	−0.8 (3)
Cd—S2—C1—S1	2.29 (8)	N5—C17—C18—C14	0.1 (3)
Cd—S1—C1—N1	178.07 (12)	C15—C14—C18—C17	0.9 (3)
Cd—S1—C1—S2	−2.31 (8)	C13—C14—C18—C17	−179.34 (16)
C1—N1—C2—C3	91.28 (18)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1o···$N5^{ii}$	0.84 (2)	1.98 (2)	2.810 (2)	176 (2)

C10—H10···O1^{iii}	0.95	2.55	3.480 (3)	168
C3—H3a···N4^{iv}	0.99	2.61	3.369 (3)	134

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

Fig. 1

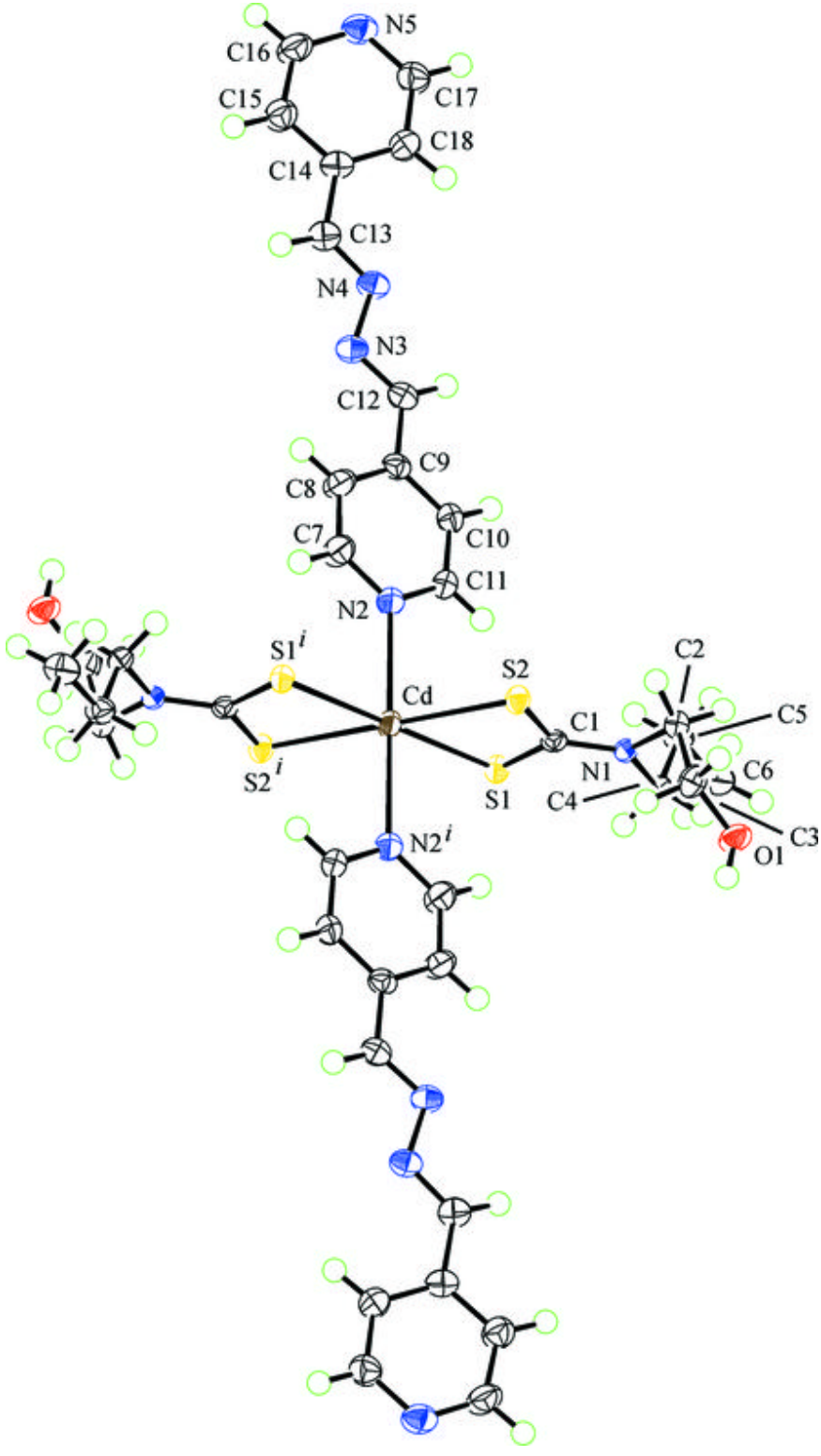
N5
C16
C15
C17
C18
C14
C13
N4
N3
C12
C9
C8
C7
C10
C11
N2
S1^{i}
S2
Cd
C1
C2
C5
N1
C6
C4
S2^{i}
S1
N2^{i}
O1
C3

Fig. 2

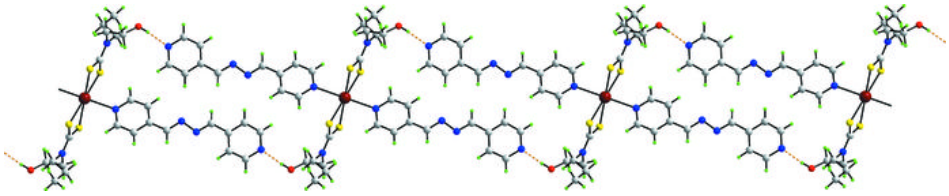

Fig. 3