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Poly[[μ_3-4-(4,5-diazafluoren-9-ylideneamino)benzoato-$\kappa^3O,O':N$](methanol-κO)(thiocyanato-κN)cadmium(II)]

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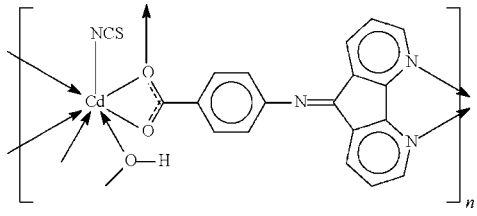
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.073; data-to-parameter ratio = 18.1.

In the crystal structure of the title compound, $[Cd(C_{18}H_{10}NO_2)(NCS)(CH_3OH)]_n$, the Cd^{II} atom is O,O'-chelated by the monoanionic carboxylate group and N,N'-chelated by the diazafluorene portion of a symmetry-related ligand. The geometry is seven-coordinate pentagonal bipyramidal. The crystal structure exhibits intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Wang *et al.* (1998); Xiao *et al.* (2000); Xu *et al.* (2003).



Experimental

Crystal data

$[Cd(C_{18}H_{10}NO_2)(NCS)(CH_4O)]$
M_r = 502.81
Monoclinic, $P2_1/c$
a = 8.3118 (7) Å
b = 8.8422 (7) Å
c = 26.829 (2) Å
β = 98.193 (1)°
V = 1951.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 291 (2) K
0.28 × 0.18 × 0.11 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.718, T_{max} = 0.871
17426 measured reflections
4767 independent reflections
4054 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.073
S = 1.00
4767 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N4	2.219 (3)	Cd1—O2^{ii}	2.4466 (19)
Cd1—O3	2.314 (2)	Cd1—O2	2.5027 (17)
Cd1—N1^{i}	2.394 (2)	Cd1—N2^{i}	2.6161 (19)
Cd1—O1	2.4351 (19)		
N4—Cd1—O3	106.34 (9)	O3—Cd1—O2	98.71 (6)
N4—Cd1—N1^{i}	147.31 (8)	N1^{i}—Cd1—O2	78.99 (6)
O3—Cd1—N1^{i}	84.96 (7)	O1—Cd1—O2	52.57 (6)
N4—Cd1—O1	87.08 (8)	O2^{ii}—Cd1—O2	72.34 (7)
O3—Cd1—O1	79.96 (7)	N4—Cd1—N2^{i}	80.35 (8)
N1^{i}—Cd1—O1	125.45 (7)	O3—Cd1—N2^{i}	77.79 (7)
N4—Cd1—O2^{ii}	87.65 (9)	N1^{i}—Cd1—N2^{i}	72.08 (6)
O3—Cd1—O2^{ii}	165.99 (7)	O1—Cd1—N2^{i}	150.11 (7)
N1^{i}—Cd1—O2^{ii}	82.77 (7)	O2^{ii}—Cd1—N2^{i}	104.65 (6)
O1—Cd1—O2^{ii}	101.78 (6)	O2—Cd1—N2^{i}	151.04 (7)
N4—Cd1—O2	127.41 (7)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O1^{iii}	0.82	1.85	2.658 (3)	169

Symmetry code: (iii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT* (Bruker 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: NG2247).

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supplementary materials

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Poly[[μ_3-4-(4,5-diazafluoren-9-ylideneamino)benzoato-$\kappa^3O,O':N$](methanol-κO)(thiocyanato-κN)cadmium(II)]

J.-M. Zheng, C.-X. Du and Y.-J. Wu

Comment

4,5-Diazafluorene-9-one and its derivatives are excellent chelating agents (Wang *et al.*, 1998; Xiao *et al.*, 2000; Xu *et al.*, 2003). 4-(4,5-Diazafluoren-9-ylidieneamino)benzoic acid possesses a carboxylic acid substituent, and is then capable of binding through both the diazafluorene as well as the carboxyl parts of the deprotonated carboxylic acid.

In the crystal structure of the title complex (I), the Cd^{II} atom shows pentagonal bipyramid coordination. The carboxylate group functions in μ_3 bridging mode; it chelates to two metal atoms through the carboxyl and diazafluorene parts and additionally, it uses the oxygen atom of the carboxyl portion to interact with a third metal atom (Fig. 1). Such a bridging mode gives rise to a layer. The coordinated methanol molecular engages in a hydrogen bonding interaction to lead to a three-dimensional hydrogen-bonded structure.

Experimental

The dafb compound was synthesized by the condensation of 4,5-diazafluorene-9-one with 4-amino-benzoic acid in 1:1 molar ratio in anhydrous ethanol. The title complex was prepared by the reaction of $Cd(NO_3)_2{\cdot}4H_2O$ (0.308 g, 1.0 mmol), NaSCN (0.081 g, 1.0 mmol) and acid (0.301 g, 1.0 mmol) in 50 ml me thanol; the solution was heated for 2 h. Light yellow crystals were obtained by slow evaporation of the solvent.

Refinement

H atom bonded to O atom was located in a difference map and refined with O—H = 0.82 Å, and with U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

Figures

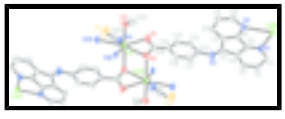


Fig. 1. The structure of the title complex showing the atom-numbering scheme.

Poly[[μ_3-4-(4,5-diazafluoren-9-ylideneamino)benzoato- $\kappa^3O,O^1:N$](methanol-κO)(thiocyanoato-κN)cadmium(II)]

Crystal data

$[Cd(C_{18}H_{10}N_1O_2)(NCS)(CH_4O)]$	$F_{000} = 1000$
$M_r = 502.81$	$D_x = 1.711$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6196 reflections
$a = 8.3118$ (7) Å	$\theta = 2.4$–28.0º
$b = 8.8422$ (7) Å	$\mu = 1.26$ mm^{-1}
$c = 26.829$ (2) Å	$T = 291$ (2) K
$\beta = 98.1930$ (10)º	Block, yellow
$V = 1951.7$ (3) Å^3	0.28 × 0.18 × 0.11 mm
$Z = 4$	

Data collection

Bruker SMART CCD area detector diffractometer	4767 independent reflections
Radiation source: fine-focus sealed tube	4054 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 291(2)$ K	$\theta_{max} = 28.2$º
φ and ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -11 \rightarrow 11$
$T_{min} = 0.718$, $T_{max} = 0.871$	$k = -11 \rightarrow 11$
17426 measured reflections	$l = -35 \rightarrow 35$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters not refined
$wR(F^2) = 0.073$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 1.156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.002$
4767 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
263 parameters	$\Delta\rho_{min} = -0.80$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
Cd1	0.70919 (2)	0.48390 (2)	0.546677 (6)	0.03675 (7)
S1	0.95499 (18)	0.93208 (14)	0.63347 (4)	0.1048 (4)
O1	0.7890 (2)	0.5393 (3)	0.46472 (7)	0.0523 (5)
O2	0.5646 (2)	0.4085 (2)	0.46208 (6)	0.0444 (4)
O3	0.9340 (2)	0.3282 (2)	0.54939 (7)	0.0519 (5)
H3O	1.0209	0.3718	0.5490	0.078*
N1	0.5713 (2)	0.2399 (2)	0.06768 (6)	0.0354 (4)
N2	0.7869 (3)	0.0638 (3)	0.14334 (7)	0.0401 (5)
N3	0.5485 (3)	0.4793 (3)	0.22597 (8)	0.0481 (6)
N4	0.8030 (3)	0.7114 (3)	0.57061 (9)	0.0597 (7)
C1	0.4633 (3)	0.3307 (3)	0.04010 (9)	0.0427 (6)
H1	0.4402	0.3137	0.0056	0.051*
C2	0.3851 (4)	0.4483 (3)	0.06077 (10)	0.0495 (7)
H2	0.3110	0.5076	0.0401	0.059*
C3	0.4157 (4)	0.4792 (3)	0.11212 (10)	0.0462 (6)
H3	0.3618	0.5562	0.1266	0.055*
C4	0.5301 (3)	0.3895 (3)	0.14043 (8)	0.0372 (5)
C5	0.6003 (3)	0.2731 (3)	0.11655 (8)	0.0332 (5)
C6	0.7071 (3)	0.1857 (3)	0.15418 (8)	0.0344 (5)
C7	0.7030 (3)	0.2487 (3)	0.20194 (8)	0.0352 (5)
C8	0.7956 (3)	0.1783 (3)	0.24217 (9)	0.0439 (6)
H8	0.7994	0.2147	0.2748	0.053*
C9	0.8828 (4)	0.0508 (3)	0.23184 (10)	0.0497 (7)
H9	0.9475	0.0012	0.2580	0.060*
C10	0.8745 (4)	−0.0036 (3)	0.18286 (10)	0.0488 (7)
H10	0.9324	−0.0906	0.1774	0.059*
C11	0.5921 (3)	0.3827 (3)	0.19545 (8)	0.0375 (5)
C12	0.5947 (3)	0.4675 (3)	0.27888 (9)	0.0414 (6)
C13	0.7029 (3)	0.5695 (3)	0.30414 (9)	0.0444 (6)
H13	0.7547	0.6397	0.2861	0.053*
C14	0.7345 (3)	0.5677 (3)	0.35641 (9)	0.0430 (6)
H14	0.8113	0.6333	0.3732	0.052*
C15	0.6512 (3)	0.4675 (3)	0.38363 (8)	0.0352 (5)

C16	0.5414 (3)	0.3666 (3)	0.35808 (9)	0.0427 (6)
H16	0.4856	0.2996	0.3761	0.051*
C17	0.5141 (4)	0.3645 (3)	0.30582 (9)	0.0483 (6)
H17	0.4423	0.2947	0.2889	0.058*
C18	0.6715 (3)	0.4716 (3)	0.43996 (9)	0.0379 (5)
C19	0.8661 (4)	0.8014 (3)	0.59673 (10)	0.0527 (7)
C20	0.9307 (4)	0.1948 (4)	0.52030 (14)	0.0719 (9)
H20A	0.8645	0.1203	0.5337	0.108*
H20B	1.0392	0.1566	0.5213	0.108*
H20C	0.8860	0.2169	0.4861	0.108*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03888 (11)	0.04895 (12)	0.02229 (9)	−0.00736 (8)	0.00388 (7)	0.00269 (7)
S1	0.1406 (11)	0.0846 (7)	0.0753 (7)	−0.0278 (7)	−0.0325 (7)	−0.0164 (6)
O1	0.0524 (12)	0.0758 (13)	0.0274 (8)	−0.0102 (10)	0.0012 (8)	−0.0017 (8)
O2	0.0512 (11)	0.0575 (11)	0.0263 (8)	0.0008 (9)	0.0115 (7)	0.0070 (8)
O3	0.0420 (10)	0.0662 (13)	0.0472 (10)	−0.0041 (9)	0.0050 (8)	−0.0049 (9)
N1	0.0417 (11)	0.0454 (11)	0.0190 (8)	−0.0020 (9)	0.0041 (8)	−0.0035 (7)
N2	0.0423 (12)	0.0493 (12)	0.0292 (10)	0.0053 (10)	0.0068 (8)	−0.0049 (9)
N3	0.0696 (16)	0.0512 (13)	0.0230 (10)	0.0145 (11)	0.0043 (10)	−0.0049 (9)
N4	0.0773 (18)	0.0629 (16)	0.0371 (12)	−0.0212 (14)	0.0015 (12)	−0.0017 (11)
C1	0.0541 (16)	0.0492 (15)	0.0232 (11)	−0.0006 (12)	0.0002 (10)	−0.0007 (10)
C2	0.0613 (18)	0.0505 (15)	0.0333 (13)	0.0104 (13)	−0.0052 (12)	0.0029 (11)
C3	0.0586 (17)	0.0446 (14)	0.0346 (13)	0.0108 (12)	0.0035 (12)	−0.0030 (10)
C4	0.0477 (14)	0.0412 (13)	0.0225 (10)	−0.0008 (11)	0.0046 (9)	−0.0015 (9)
C5	0.0374 (12)	0.0408 (12)	0.0218 (10)	−0.0036 (10)	0.0057 (9)	−0.0010 (9)
C6	0.0360 (12)	0.0444 (13)	0.0231 (10)	−0.0012 (10)	0.0055 (9)	−0.0019 (9)
C7	0.0388 (13)	0.0449 (13)	0.0222 (10)	−0.0009 (10)	0.0055 (9)	−0.0026 (9)
C8	0.0482 (15)	0.0579 (16)	0.0246 (11)	0.0038 (12)	0.0021 (10)	−0.0023 (10)
C9	0.0499 (16)	0.0644 (18)	0.0325 (13)	0.0128 (14)	−0.0021 (11)	0.0015 (12)
C10	0.0482 (15)	0.0586 (17)	0.0390 (14)	0.0134 (13)	0.0042 (12)	−0.0037 (11)
C11	0.0463 (14)	0.0435 (13)	0.0224 (10)	0.0012 (11)	0.0036 (9)	−0.0019 (9)
C12	0.0541 (15)	0.0477 (14)	0.0226 (10)	0.0152 (12)	0.0064 (10)	−0.0059 (9)
C13	0.0458 (15)	0.0603 (16)	0.0284 (12)	0.0017 (12)	0.0102 (10)	0.0059 (11)
C14	0.0405 (14)	0.0609 (16)	0.0273 (11)	−0.0045 (12)	0.0044 (10)	0.0000 (11)
C15	0.0389 (12)	0.0459 (13)	0.0213 (10)	0.0064 (10)	0.0062 (9)	−0.0006 (9)
C16	0.0571 (16)	0.0412 (13)	0.0311 (12)	−0.0005 (12)	0.0110 (11)	−0.0016 (10)
C17	0.0671 (18)	0.0434 (14)	0.0330 (13)	−0.0008 (13)	0.0020 (12)	−0.0095 (11)
C18	0.0446 (14)	0.0451 (13)	0.0245 (11)	0.0064 (11)	0.0070 (10)	0.0012 (9)
C19	0.0621 (18)	0.0596 (18)	0.0344 (13)	−0.0082 (14)	0.0001 (12)	0.0070 (12)
C20	0.066 (2)	0.068 (2)	0.083 (2)	−0.0048 (17)	0.0171 (19)	−0.0144 (18)

Geometric parameters (Å, °)

Cd1—N4	2.219 (3)	C3—H3	0.9300
Cd1—O3	2.314 (2)	C4—C5	1.385 (3)

Cd1—N1^{i}	2.394 (2)	C4—C11	1.494 (3)
Cd1—O1	2.4351 (19)	C5—C6	1.466 (3)
Cd1—O2^{ii}	2.4466 (19)	C6—C7	1.402 (3)
Cd1—O2	2.5027 (17)	C7—C8	1.382 (3)
Cd1—N2^{i}	2.6161 (19)	C7—C11	1.496 (3)
S1—C19	1.626 (3)	C8—C9	1.389 (4)
O1—C18	1.252 (3)	C8—H8	0.9300
O2—C18	1.266 (3)	C9—C10	1.392 (4)
O2—Cd1^{ii}	2.4466 (18)	C9—H9	0.9300
O3—C20	1.412 (4)	C10—H10	0.9300
O3—H3O	0.8200	C12—C13	1.381 (4)
N1—C5	1.332 (3)	C12—C17	1.393 (4)
N1—C1	1.345 (3)	C13—C14	1.390 (3)
N1—Cd1^{iii}	2.394 (2)	C13—H13	0.9300
N2—C6	1.319 (3)	C14—C15	1.394 (4)
N2—C10	1.338 (3)	C14—H14	0.9300
N2—Cd1^{iii}	2.6161 (19)	C15—C16	1.386 (4)
N3—C11	1.272 (3)	C15—C18	1.497 (3)
N3—C12	1.421 (3)	C16—C17	1.388 (3)
N4—C19	1.138 (4)	C16—H16	0.9300
C1—C2	1.384 (4)	C17—H17	0.9300
C1—H1	0.9300	C20—H20A	0.9600
C2—C3	1.392 (4)	C20—H20B	0.9600
C2—H2	0.9300	C20—H20C	0.9600
C3—C4	1.380 (4)		
N4—Cd1—O3	106.34 (9)	N1—C5—C6	124.7 (2)
N4—Cd1—N1^{i}	147.31 (8)	C4—C5—C6	109.10 (19)
O3—Cd1—N1^{i}	84.96 (7)	N2—C6—C7	127.2 (2)
N4—Cd1—O1	87.08 (8)	N2—C6—C5	123.57 (19)
O3—Cd1—O1	79.96 (7)	C7—C6—C5	109.2 (2)
N1^{i}—Cd1—O1	125.45 (7)	C8—C7—C6	116.8 (2)
N4—Cd1—O2^{ii}	87.65 (9)	C8—C7—C11	135.5 (2)
O3—Cd1—O2^{ii}	165.99 (7)	C6—C7—C11	107.66 (19)
N1^{i}—Cd1—O2^{ii}	82.77 (7)	C7—C8—C9	117.3 (2)
O1—Cd1—O2^{ii}	101.78 (6)	C7—C8—H8	121.4
N4—Cd1—O2	127.41 (7)	C9—C8—H8	121.4
O3—Cd1—O2	98.71 (6)	C8—C9—C10	120.8 (2)
N1^{i}—Cd1—O2	78.99 (6)	C8—C9—H9	119.6
O1—Cd1—O2	52.57 (6)	C10—C9—H9	119.6
O2^{ii}—Cd1—O2	72.34 (7)	N2—C10—C9	122.8 (2)
N4—Cd1—N2^{i}	80.35 (8)	N2—C10—H10	118.6
O3—Cd1—N2^{i}	77.79 (7)	C9—C10—H10	118.6
N1^{i}—Cd1—N2^{i}	72.08 (6)	N3—C11—C4	121.3 (2)
O1—Cd1—N2^{i}	150.11 (7)	N3—C11—C7	133.2 (2)
O2^{ii}—Cd1—N2^{i}	104.65 (6)	C4—C11—C7	105.50 (19)

O2—Cd1—N2^{i}	151.04 (7)	C13—C12—C17	120.0 (2)
C18—O1—Cd1	95.20 (15)	C13—C12—N3	120.4 (2)
C18—O2—Cd1^{ii}	119.27 (16)	C17—C12—N3	119.0 (2)
C18—O2—Cd1	91.66 (14)	C12—C13—C14	120.3 (2)
Cd1^{ii}—O2—Cd1	107.66 (7)	C12—C13—H13	119.9
C20—O3—Cd1	121.83 (19)	C14—C13—H13	119.9
C20—O3—H3O	109.5	C13—C14—C15	120.0 (2)
Cd1—O3—H3O	115.4	C13—C14—H14	120.0
C5—N1—C1	115.0 (2)	C15—C14—H14	120.0
C5—N1—Cd1^{iii}	112.84 (15)	C16—C15—C14	119.4 (2)
C1—N1—Cd1^{iii}	131.95 (15)	C16—C15—C18	119.1 (2)
C6—N2—C10	115.0 (2)	C14—C15—C18	121.4 (2)
C6—N2—Cd1^{iii}	106.82 (15)	C15—C16—C17	120.7 (2)
C10—N2—Cd1^{iii}	138.01 (17)	C15—C16—H16	119.7
C11—N3—C12	122.2 (2)	C17—C16—H16	119.7
C19—N4—Cd1	157.6 (2)	C16—C17—C12	119.6 (2)
N1—C1—C2	122.9 (2)	C16—C17—H17	120.2
N1—C1—H1	118.5	C12—C17—H17	120.2
C2—C1—H1	118.5	O1—C18—O2	120.6 (2)
C1—C2—C3	120.9 (2)	O1—C18—C15	120.9 (2)
C1—C2—H2	119.5	O2—C18—C15	118.5 (2)
C3—C2—H2	119.5	N4—C19—S1	179.1 (3)
C4—C3—C2	116.5 (2)	O3—C20—H20A	109.5
C4—C3—H3	121.7	O3—C20—H20B	109.5
C2—C3—H3	121.7	H20A—C20—H20B	109.5
C3—C4—C5	118.4 (2)	O3—C20—H20C	109.5
C3—C4—C11	132.9 (2)	H20A—C20—H20C	109.5
C5—C4—C11	108.6 (2)	H20B—C20—H20C	109.5
N1—C5—C4	126.2 (2)		
N4—Cd1—O1—C18	−144.23 (18)	Cd1^{iii}—N2—C6—C5	−1.2 (3)
O3—Cd1—O1—C18	108.61 (17)	N1—C5—C6—N2	0.1 (4)
N1^{i}—Cd1—O1—C18	32.23 (19)	C4—C5—C6—N2	177.4 (2)
O2^{ii}—Cd1—O1—C18	−57.24 (17)	N1—C5—C6—C7	−177.3 (2)
O2—Cd1—O1—C18	−0.61 (15)	C4—C5—C6—C7	0.0 (3)
N2^{i}—Cd1—O1—C18	150.96 (16)	N2—C6—C7—C8	1.7 (4)
N4—Cd1—O2—C18	48.83 (18)	C5—C6—C7—C8	179.0 (2)
O3—Cd1—O2—C18	−69.56 (15)	N2—C6—C7—C11	−178.1 (2)
N1^{i}—Cd1—O2—C18	−152.65 (15)	C5—C6—C7—C11	−0.8 (3)
O1—Cd1—O2—C18	0.60 (14)	C6—C7—C8—C9	−0.7 (4)
O2^{ii}—Cd1—O2—C18	121.51 (17)	C11—C7—C8—C9	179.1 (3)
N2^{i}—Cd1—O2—C18	−150.06 (16)	C7—C8—C9—C10	−0.8 (4)
N4—Cd1—O2—Cd1^{ii}	−72.68 (12)	C6—N2—C10—C9	−0.6 (4)
O3—Cd1—O2—Cd1^{ii}	168.93 (7)	Cd1^{iii}—N2—C10—C9	−176.0 (2)
N1^{i}—Cd1—O2—Cd1^{ii}	85.84 (7)	C8—C9—C10—N2	1.5 (5)
O1—Cd1—O2—Cd1^{ii}	−120.91 (10)	C12—N3—C11—C4	174.4 (2)

O2^{ii}—Cd1—O2—Cd1^{ii}	0.0	C12—N3—C11—C7	−5.6 (5)
N2^{i}—Cd1—O2—Cd1^{ii}	88.43 (14)	C3—C4—C11—N3	−5.9 (5)
N4—Cd1—O3—C20	−156.4 (2)	C5—C4—C11—N3	178.8 (2)
N1^{i}—Cd1—O3—C20	54.9 (2)	C3—C4—C11—C7	174.2 (3)
O1—Cd1—O3—C20	−72.4 (2)	C5—C4—C11—C7	−1.2 (3)
O2^{ii}—Cd1—O3—C20	26.0 (4)	C8—C7—C11—N3	1.5 (5)
O2—Cd1—O3—C20	−23.1 (2)	C6—C7—C11—N3	−178.8 (3)
N2^{i}—Cd1—O3—C20	127.7 (2)	C8—C7—C11—C4	−178.5 (3)
O3—Cd1—N4—C19	−63.6 (7)	C6—C7—C11—C4	1.2 (3)
N1^{i}—Cd1—N4—C19	43.0 (8)	C11—N3—C12—C13	110.8 (3)
O1—Cd1—N4—C19	−142.3 (7)	C11—N3—C12—C17	−77.4 (4)
O2^{ii}—Cd1—N4—C19	115.8 (7)	C17—C12—C13—C14	1.5 (4)
O2—Cd1—N4—C19	−178.7 (7)	N3—C12—C13—C14	173.1 (2)
N2^{i}—Cd1—N4—C19	10.5 (7)	C12—C13—C14—C15	−3.1 (4)
C5—N1—C1—C2	−1.2 (4)	C13—C14—C15—C16	2.3 (4)
Cd1^{iii}—N1—C1—C2	173.6 (2)	C13—C14—C15—C18	−174.6 (2)
N1—C1—C2—C3	0.3 (5)	C14—C15—C16—C17	0.0 (4)
C1—C2—C3—C4	1.7 (4)	C18—C15—C16—C17	177.1 (2)
C2—C3—C4—C5	−2.6 (4)	C15—C16—C17—C12	−1.7 (4)
C2—C3—C4—C11	−177.7 (3)	C13—C12—C17—C16	0.9 (4)
C1—N1—C5—C4	0.1 (4)	N3—C12—C17—C16	−170.9 (2)
Cd1^{iii}—N1—C5—C4	−175.67 (19)	Cd1—O1—C18—O2	1.1 (3)
C1—N1—C5—C6	177.0 (2)	Cd1—O1—C18—C15	179.1 (2)
Cd1^{iii}—N1—C5—C6	1.2 (3)	Cd1^{ii}—O2—C18—O1	110.3 (2)
C3—C4—C5—N1	1.9 (4)	Cd1—O2—C18—O1	−1.1 (3)
C11—C4—C5—N1	178.0 (2)	Cd1^{ii}—O2—C18—C15	−67.8 (3)
C3—C4—C5—C6	−175.4 (2)	Cd1—O2—C18—C15	−179.1 (2)
C11—C4—C5—C6	0.8 (3)	C16—C15—C18—O1	166.5 (2)
C10—N2—C6—C7	−1.0 (4)	C14—C15—C18—O1	−16.5 (4)
Cd1^{iii}—N2—C6—C7	175.7 (2)	C16—C15—C18—O2	−15.4 (4)
C10—N2—C6—C5	−178.0 (2)	C14—C15—C18—O2	161.5 (2)

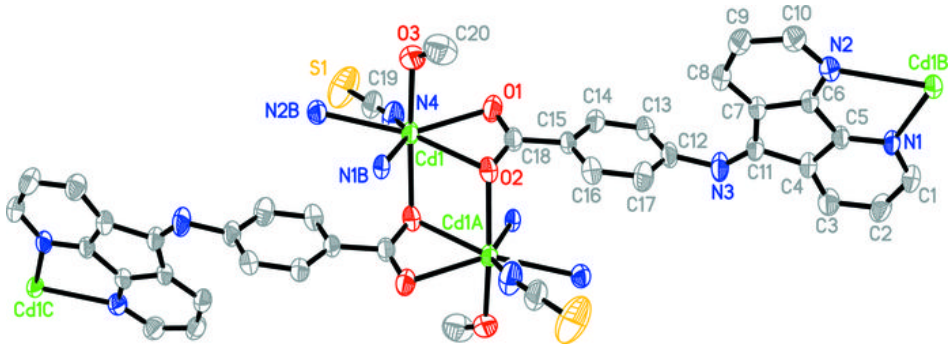
Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3O···O1^{iv}	0.82	1.85	2.658 (3)	169

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

Fig. 1


O3
C20
S1
C19
N2B
N4
O1
C15
C14
C13
C12
C9
C10
N2
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C8
C7
C6
C5
N1
C1
C2
C3
C4
C11
N3
C16
C17
C18
N1B
Cd1
O2
Cd1A
Cd1C