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catena-Poly[[[diiodidocadmium(II)]-μ-1-(4-pyridylmethyl)-1*H*-benzimidazole] methanol hemisolvate]

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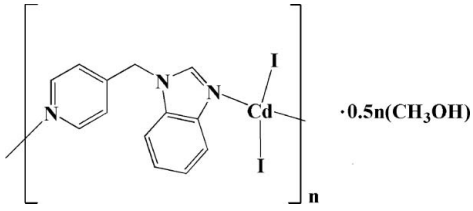
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.024; wR factor = 0.054; data-to-parameter ratio = 16.3.

In the title coordination polymer, $\{[CdI_2(C_{13}H_{11}N_3)]\cdot 0.5CH_4O\}_n$, each Cd^{II} center is four-coordinated by two N-atom donors from two 1-(4-pyridylmethyl)-1*H*-benzimidazole (*L*) ligands and two iodide anions, forming a tetrahedral coordination geometry. *L* ligands bridge adjacent Cd^{II} ions, generating two crystallographically independent approximately orthogonal one-dimensional chains. The methanol solvent molecule associates with one of the chains *via* O—H···I interactions.

Related literature

For a review of *N*-containing heterocyclic aromatic compounds as bridging ligands, see: Steel (2005). For a discussion of benzimidazole ligands in complexes, see: Li *et al.* (2007); Meng *et al.* (2004). For an example of a silver coordination polymer of the present ligand, see: Huang *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[CdI_2(C_{13}H_{11}N_3)]\cdot 0.5CH_4O$
M_r = 591.47
Monoclinic, $P2_1/c$
a = 17.469 (4) Å
b = 12.913 (3) Å
c = 16.814 (3) Å
β = 117.56 (3)°
V = 3362.6 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.97 mm^{-1}
T = 293 (2) K
0.10 × 0.06 × 0.04 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.637, T_{max} = 0.826
33513 measured reflections
5901 independent reflections
5155 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.054
S = 1.02
5901 reflections
363 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3^{i}	2.271 (3)	Cd2—N6^{ii}	2.236 (3)
Cd1—N1	2.278 (3)	Cd2—N4	2.315 (3)
Cd1—I2	2.7051 (6)	Cd2—I3	2.702 (6)
Cd1—I1	2.7264 (10)	Cd2—I4	2.706 (1)
N3^{i}—Cd1—N1	97.99 (11)	N6^{ii}—Cd2—N4	98.86 (12)
N3^{i}—Cd1—I2	108.01 (8)	N6^{ii}—Cd2—I3	107.34 (9)
N1—Cd1—I2	106.72 (8)	N4—Cd2—I3	105.01 (8)
N3^{i}—Cd1—I1	104.48 (8)	N6^{ii}—Cd2—I4	110.99 (9)
N1—Cd1—I1	106.76 (8)	N4—Cd2—I4	100.80 (8)
I2—Cd1—I1	128.711 (15)	I3—Cd2—I4	129.14 (8)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···I2^{iii}	0.82	2.88	3.647 (5)	155

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear* (Rigaku/MSC, 2005); data reduction: *CrystalClear* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SQ2002).

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supporting information

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catena-Poly[[[diiodidocadmium(II)]-μ-1-(4-pyridylmethyl)-1*H*-benzimidazole] methanol hemisolvate]

Jun-Jie Wang, Li-Fan Yan and Tong-Liang Hu

S1. Comment

N-containing heterocyclic aromatic compounds are extensively used as bridging ligands in coordination and metallosupramolecular chemistry (Steel, 2005). In recent years, benzimidazole groups have been used to link different alkyl or aromatic groups to form a series of bi- and multi-dentate flexible ligands, which can adopt different conformations according to the different geometric requirements of the metal centers when forming complexes (Li *et al.*, 2007). Many complexes with these ligands show unique structural topologies and interesting properties (Meng *et al.*, 2004). Recently, Liu and co-workers synthesized a flexible bridging ligand 1-(pyridin-4-ylmethyl)-1*H*-benzo[*d*]imidazole (*L*) as well as its chiral one-dimensional double helix polymer, $[Ag(L)(NO_3)]_n$ (Huang *et al.*, 2006). We herein report the crystal structure of a cadmium complex of this ligand (I).

In the molecule of (I), (Fig. 1 and 2), the bond lengths and angles (Table 1) are generally within normal ranges (Allen *et al.*, 1987). The Cd^{II} center is tetrahedrally coordinated by two N atoms from two *L* ligands (*L* = 1-(pyridin-4-yl-methyl)-1*H*-benzo[*d*]imidazole) and two iodide ions. In the extended structure of (I), the Cd^{II} centers are interconnected by *L* ligands to form two one-dimensional chains along two different directions (Fig. 3). The chain containing Cd1 is along the *c* direction and the other one containing Cd2 is along the *b* direction, making them essentially orthogonal. The methanol solvate molecules are associated with the Cd1 chains *via* O—H···I interactions.

S2. Experimental

The ligand 1-(pyridin-4-ylmethyl)-1*H*-benzo[*d*]imidazole (*L*) was synthesized according to a reported method (Li *et al.*, 2007). The reaction of *L* (58 mg, 0.2 mmol), NaI (30 mg, 0.2 mmol) and $Cd(ClO_4)_2$ (31 mg, 0.1 mmol) in a solution of methanol and water (*v*/*v* = 1:1,10 ml) for a few minutes afforded a white solid, which was separated by filtration. The resulting solution was kept at room temperature. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of the solvent after several days (yield: 40%).

S3. Refinement

H atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 (aromatic) and 0.97 Å (methylene) and U_{iso}(H) = 1.2*U_{eq}(C).

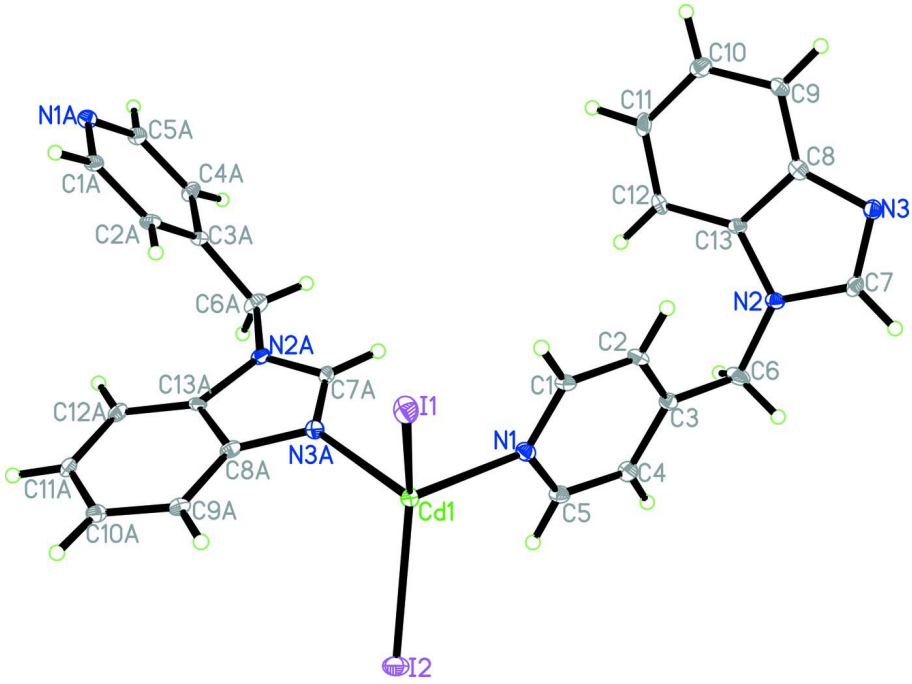

Figure 1

The coordination environment of Cd1, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry code: (A) *x*, 3/2 - *y*, 1/2 + *z*].

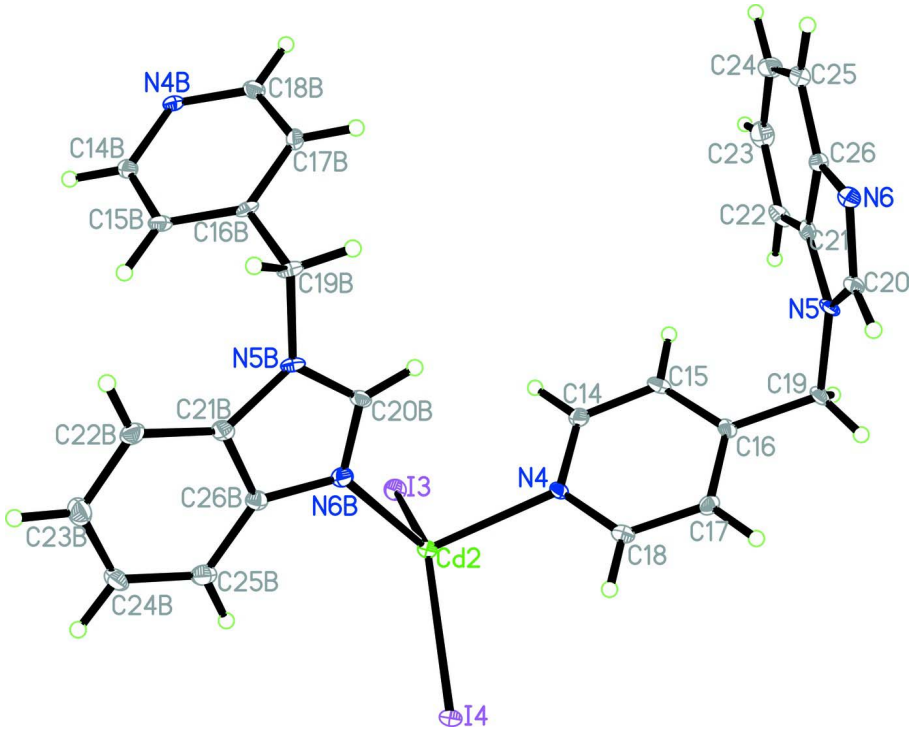

Figure 2

The coordination environment of Cd2, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. [symmetry code: (B) 1 - *x*, -1/2 + *y*, 3/2 - *z*].

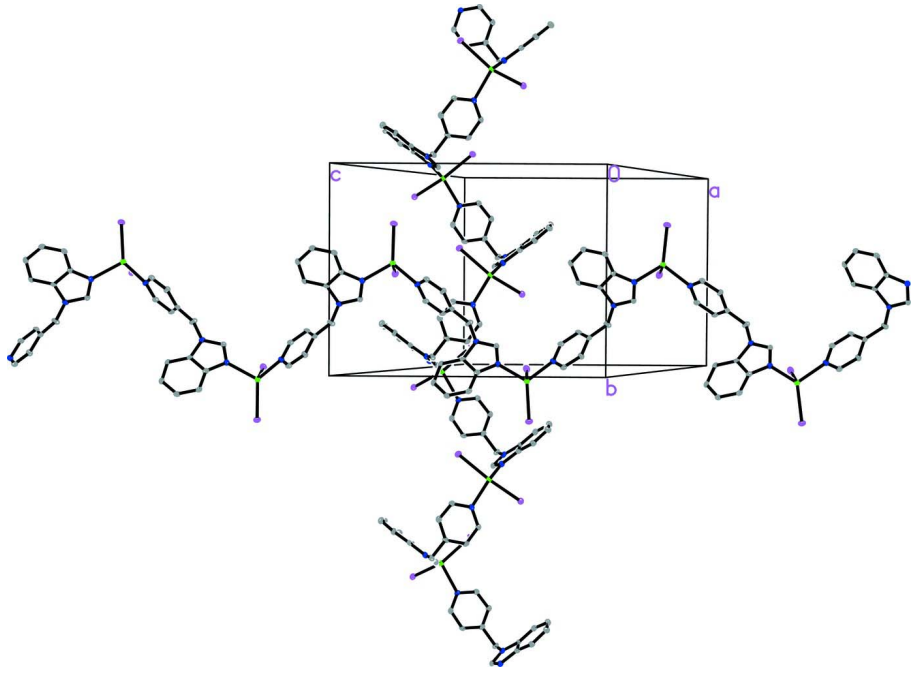

Figure 3

View of the two crystallographically independent one-dimensional chains that run along the *b* and *c* axes.

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Crystal data

$[CdI_2(C_{13}H_{11}N_3)]\cdot 0.5CH_4O$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.469\ (4)$ Å
$b = 12.913\ (3)$ Å
$c = 16.814\ (3)$ Å
$\beta = 117.56\ (3)°$
$V = 3362.6\ (16)$ Å^3
$Z = 8$
$F(000) = 2184$
$D_x = 2.337$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9593 reflections
$\theta = 2.7–25.0°$
$\mu = 4.97$ mm^{-1}
$T = 293$ K
Block, colorless
0.10 × 0.06 × 0.04 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.637$, $T_{max} = 0.826$
33513 measured reflections
5901 independent reflections
5155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.066$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -20\rightarrow20$
$k = -15\rightarrow15$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.054$
$S = 1.02$
5901 reflections
363 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
$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.49$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.185504 (19)	0.46826 (2)	0.868473 (19)	0.01644 (8)
Cd2	0.272027 (19)	0.52226 (2)	0.547057 (19)	0.01630 (8)
I1	0.356936 (18)	0.51615 (2)	0.948024 (19)	0.02392 (8)
I2	0.109810 (19)	0.27969 (2)	0.825044 (19)	0.02452 (8)
I3	0.2197 (2)	0.3922 (2)	0.6382 (2)	0.0220 (8)
I4	0.178051 (18)	0.61285 (2)	0.385404 (17)	0.02101 (8)
N1	0.1207 (2)	0.5680 (2)	0.7429 (2)	0.0166 (8)
N2	0.0638 (2)	0.8382 (2)	0.4991 (2)	0.0158 (8)
N3	0.1338 (2)	0.9484 (3)	0.4526 (2)	0.0169 (8)
N4	0.32450 (19)	0.6665 (2)	0.6382 (2)	0.0142 (8)
N5	0.4629 (2)	0.9308 (2)	0.8829 (2)	0.0159 (8)
N6	0.6033 (2)	0.9608 (3)	0.9407 (2)	0.0178 (8)
C1	0.1638 (2)	0.6488 (3)	0.7339 (3)	0.0159 (9)
H1A	0.2159	0.6671	0.7826	0.019*
C2	0.1355 (2)	0.7062 (3)	0.6570 (3)	0.0160 (9)
H2A	0.1694	0.7594	0.6531	0.019*
C3	0.0561 (3)	0.6843 (3)	0.5853 (3)	0.0155 (9)
C4	0.0106 (3)	0.5992 (3)	0.5937 (3)	0.0190 (10)
H4A	−0.0423	0.5802	0.5464	0.023*
C5	0.0448 (3)	0.5442 (3)	0.6721 (3)	0.0171 (9)
H5A	0.0141	0.4877	0.6767	0.020*
C6	0.0143 (3)	0.7484 (3)	0.5008 (3)	0.0236 (10)
H6A	0.0044	0.7044	0.4501	0.028*
H6B	−0.0415	0.7718	0.4928	0.028*
C7	0.0926 (2)	0.8603 (3)	0.4385 (3)	0.0167 (9)
H7A	0.0837	0.8165	0.3911	0.020*
C8	0.1326 (2)	0.9898 (3)	0.5286 (3)	0.0152 (9)
C13	0.0877 (2)	0.9230 (3)	0.5583 (3)	0.0135 (9)
C12	0.0736 (3)	0.9453 (3)	0.6317 (3)	0.0175 (10)

H12A	0.0428	0.9009	0.6499	0.021*
C11	0.1082 (3)	1.0372 (3)	0.6757 (3)	0.0220 (10)
H11A	0.0999	1.0559	0.7246	0.026*
C10	0.1551 (3)	1.1025 (3)	0.6488 (3)	0.0220 (10)
H10A	0.1790	1.1624	0.6816	0.026*
C9	0.1674 (3)	1.0815 (3)	0.5751 (3)	0.0186 (10)
H9A	0.1978	1.1269	0.5571	0.022*
C14	0.3534 (2)	0.6536 (3)	0.7270 (3)	0.0176 (9)
H14A	0.3621	0.5867	0.7500	0.021*
C15	0.3706 (2)	0.7354 (3)	0.7848 (3)	0.0191 (10)
H15A	0.3915	0.7236	0.8459	0.023*
C16	0.3568 (2)	0.8352 (3)	0.7520 (3)	0.0152 (9)
C17	0.3283 (2)	0.8485 (3)	0.6601 (3)	0.0161 (9)
H17A	0.3200	0.9147	0.6356	0.019*
C18	0.3127 (2)	0.7629 (3)	0.6064 (3)	0.0175 (10)
H18A	0.2931	0.7726	0.5452	0.021*
C19	0.3725 (2)	0.9284 (3)	0.8137 (3)	0.0174 (9)
H19A	0.3589	0.9917	0.7788	0.021*
H19B	0.3351	0.9241	0.8419	0.021*
C20	0.5281 (3)	0.9789 (3)	0.8737 (3)	0.0162 (9)
H20A	0.5194	1.0200	0.8248	0.019*
C21	0.5015 (3)	0.8769 (3)	0.9641 (3)	0.0165 (9)
C22	0.4677 (3)	0.8140 (3)	1.0078 (3)	0.0217 (10)
H22A	0.4086	0.8028	0.9843	0.026*
C23	0.5263 (3)	0.7690 (3)	1.0875 (3)	0.0273 (11)
H23A	0.5064	0.7264	1.1186	0.033*
C24	0.6145 (3)	0.7866 (3)	1.1220 (3)	0.0257 (11)
H24A	0.6522	0.7539	1.1751	0.031*
C25	0.6478 (3)	0.8505 (3)	1.0806 (3)	0.0224 (10)
H25A	0.7068	0.8631	1.1054	0.027*
C26	0.5893 (3)	0.8961 (3)	0.9996 (3)	0.0166 (9)
C27	0.4068 (3)	0.1849 (4)	0.6542 (3)	0.0435 (14)
H27A	0.4159	0.2210	0.7078	0.065*
H27B	0.3462	0.1835	0.6132	0.065*
H27C	0.4370	0.2200	0.6268	0.065*
O1	0.4380 (2)	0.0826 (2)	0.6760 (2)	0.0395 (9)
H1	0.4366	0.0545	0.6316	0.059*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01903 (18)	0.01604 (18)	0.01442 (17)	−0.00084 (13)	0.00788 (14)	0.00038 (13)
Cd2	0.01569 (17)	0.01688 (18)	0.01279 (17)	0.00087 (13)	0.00356 (14)	−0.00074 (13)
I1	0.01795 (16)	0.03018 (19)	0.01836 (16)	−0.00153 (13)	0.00393 (13)	0.00307 (13)
I2	0.02970 (18)	0.01589 (16)	0.03350 (18)	−0.00305 (13)	0.01931 (15)	−0.00410 (13)
I3	0.0239 (2)	0.0196 (2)	0.0212 (2)	−0.0028 (1)	0.0092 (1)	0.0016 (1)
I4	0.02138 (17)	0.02211 (17)	0.01193 (15)	0.00291 (12)	0.00126 (13)	0.00017 (12)
N1	0.016 (2)	0.0158 (19)	0.020 (2)	−0.0012 (15)	0.0105 (17)	0.0010 (16)

N2	0.0174 (19)	0.0115 (19)	0.0131 (18)	−0.0013 (15)	0.0024 (16)	0.0025 (15)
N3	0.018 (2)	0.017 (2)	0.0158 (19)	0.0003 (16)	0.0082 (16)	0.0001 (16)
N4	0.0109 (18)	0.017 (2)	0.0118 (18)	−0.0015 (14)	0.0023 (15)	−0.0026 (15)
N5	0.0129 (19)	0.019 (2)	0.0110 (18)	−0.0038 (15)	0.0017 (16)	−0.0074 (15)
N6	0.0146 (19)	0.021 (2)	0.0166 (19)	−0.0021 (16)	0.0060 (17)	−0.0012 (16)
C1	0.015 (2)	0.012 (2)	0.019 (2)	−0.0009 (18)	0.0061 (19)	−0.0015 (18)
C2	0.015 (2)	0.011 (2)	0.023 (2)	−0.0002 (18)	0.010 (2)	0.0030 (18)
C3	0.019 (2)	0.012 (2)	0.016 (2)	0.0034 (18)	0.0081 (19)	0.0012 (18)
C4	0.014 (2)	0.022 (3)	0.015 (2)	−0.0021 (18)	0.0015 (19)	0.0004 (19)
C5	0.016 (2)	0.016 (2)	0.018 (2)	−0.0031 (18)	0.006 (2)	−0.0014 (19)
C6	0.020 (2)	0.019 (2)	0.022 (2)	−0.009 (2)	0.002 (2)	0.002 (2)
C7	0.020 (2)	0.017 (2)	0.010 (2)	0.0059 (19)	0.0049 (19)	0.0017 (18)
C8	0.009 (2)	0.017 (2)	0.016 (2)	0.0036 (17)	0.0027 (19)	0.0048 (18)
C13	0.013 (2)	0.009 (2)	0.014 (2)	0.0031 (17)	0.0028 (18)	0.0014 (18)
C12	0.020 (2)	0.018 (2)	0.017 (2)	−0.0009 (19)	0.010 (2)	0.0047 (19)
C11	0.033 (3)	0.022 (3)	0.013 (2)	0.008 (2)	0.012 (2)	0.006 (2)
C10	0.029 (3)	0.015 (2)	0.016 (2)	0.002 (2)	0.006 (2)	0.0008 (19)
C9	0.023 (2)	0.014 (2)	0.021 (2)	0.0011 (19)	0.011 (2)	0.0048 (19)
C14	0.014 (2)	0.018 (2)	0.017 (2)	0.0009 (18)	0.0036 (19)	0.0007 (19)
C15	0.015 (2)	0.026 (3)	0.011 (2)	−0.0033 (19)	0.0015 (19)	−0.0015 (19)
C16	0.007 (2)	0.017 (2)	0.019 (2)	−0.0032 (18)	0.0026 (18)	−0.0049 (19)
C17	0.014 (2)	0.012 (2)	0.020 (2)	0.0001 (17)	0.0055 (19)	0.0048 (18)
C18	0.017 (2)	0.022 (3)	0.011 (2)	−0.0009 (19)	0.0038 (19)	0.0006 (19)
C19	0.011 (2)	0.021 (2)	0.016 (2)	−0.0028 (18)	0.0024 (19)	−0.0068 (19)
C20	0.020 (2)	0.017 (2)	0.009 (2)	0.0006 (19)	0.005 (2)	−0.0014 (18)
C21	0.023 (2)	0.015 (2)	0.011 (2)	0.0011 (19)	0.007 (2)	−0.0030 (18)
C22	0.023 (3)	0.025 (3)	0.017 (2)	−0.007 (2)	0.009 (2)	−0.006 (2)
C23	0.040 (3)	0.025 (3)	0.021 (3)	−0.003 (2)	0.017 (2)	0.000 (2)
C24	0.034 (3)	0.022 (3)	0.014 (2)	0.001 (2)	0.005 (2)	0.004 (2)
C25	0.019 (2)	0.021 (2)	0.020 (2)	0.001 (2)	0.003 (2)	−0.003 (2)
C26	0.017 (2)	0.016 (2)	0.015 (2)	0.0023 (18)	0.006 (2)	−0.0025 (18)
C27	0.041 (3)	0.042 (3)	0.041 (3)	0.006 (3)	0.014 (3)	0.005 (3)
O1	0.054 (2)	0.029 (2)	0.0241 (19)	−0.0026 (18)	0.0081 (19)	0.0014 (16)

Geometric parameters (Å, º)

Cd1—N3^{i}	2.271 (3)	C8—C13	1.405 (5)
Cd1—N1	2.278 (3)	C13—C12	1.395 (5)
Cd1—I2	2.7051 (6)	C12—C11	1.382 (5)
Cd1—I1	2.7264 (10)	C12—H12A	0.9300
Cd2—N6^{ii}	2.236 (3)	C11—C10	1.388 (5)
Cd2—N4	2.315 (3)	C11—H11A	0.9300
Cd2—I3	2.702 (6)	C10—C9	1.380 (5)
Cd2—I4	2.706 (1)	C10—H10A	0.9300
N1—C1	1.334 (5)	C9—H9A	0.9300
N1—C5	1.346 (5)	C14—C15	1.372 (5)
N2—C7	1.359 (5)	C14—H14A	0.9300
N2—C13	1.407 (5)	C15—C16	1.379 (5)

N2—C6	1.453 (5)	C15—H15A	0.9300
N3—C7	1.308 (5)	C16—C17	1.398 (5)
N3—C8	1.394 (5)	C16—C19	1.529 (5)
N3—Cd1^{iii}	2.271 (3)	C17—C18	1.373 (5)
N4—C18	1.333 (5)	C17—H17A	0.9300
N4—C14	1.347 (5)	C18—H18A	0.9300
N5—C20	1.366 (5)	C19—H19A	0.9700
N5—C21	1.397 (5)	C19—H19B	0.9700
N5—C19	1.465 (5)	C20—H20A	0.9300
N6—C20	1.297 (5)	C21—C26	1.386 (5)
N6—C26	1.401 (5)	C21—C22	1.396 (5)
N6—Cd2^{iv}	2.236 (3)	C22—C23	1.383 (6)
C1—C2	1.369 (5)	C22—H22A	0.9300
C1—H1A	0.9300	C23—C24	1.391 (6)
C2—C3	1.382 (5)	C23—H23A	0.9300
C2—H2A	0.9300	C24—C25	1.370 (5)
C3—C4	1.402 (5)	C24—H24A	0.9300
C3—C6	1.509 (5)	C25—C26	1.400 (5)
C4—C5	1.367 (5)	C25—H25A	0.9300
C4—H4A	0.9300	C27—O1	1.412 (5)
C5—H5A	0.9300	C27—H27A	0.9600
C6—H6A	0.9700	C27—H27B	0.9600
C6—H6B	0.9700	C27—H27C	0.9600
C7—H7A	0.9300	O1—H1	0.8200
C8—C9	1.394 (5)		

N3^{i}—Cd1—N1	97.99 (11)	C11—C12—H12A	122.0
N3^{i}—Cd1—I2	108.01 (8)	C13—C12—H12A	122.0
N1—Cd1—I2	106.72 (8)	C12—C11—C10	121.7 (4)
N3^{i}—Cd1—I1	104.48 (8)	C12—C11—H11A	119.2
N1—Cd1—I1	106.76 (8)	C10—C11—H11A	119.2
I2—Cd1—I1	128.711 (15)	C9—C10—C11	122.3 (4)
N6^{ii}—Cd2—N4	98.86 (12)	C9—C10—H10A	118.9
N6^{ii}—Cd2—I3	107.34 (9)	C11—C10—H10A	118.9
N4—Cd2—I3	105.01 (8)	C10—C9—C8	117.5 (4)
N6^{ii}—Cd2—I4	110.99 (9)	C10—C9—H9A	121.3
N4—Cd2—I4	100.80 (8)	C8—C9—H9A	121.3
I3—Cd2—I4	129.14 (8)	N4—C14—C15	122.5 (4)
C1—N1—C5	117.1 (3)	N4—C14—H14A	118.7
C1—N1—Cd1	118.8 (3)	C15—C14—H14A	118.7
C5—N1—Cd1	123.7 (3)	C14—C15—C16	119.7 (4)
C7—N2—C13	106.0 (3)	C14—C15—H15A	120.1
C7—N2—C6	127.6 (3)	C16—C15—H15A	120.1
C13—N2—C6	126.3 (3)	C15—C16—C17	117.7 (4)
C7—N3—C8	105.0 (3)	C15—C16—C19	121.4 (4)
C7—N3—Cd1^{iii}	130.1 (3)	C17—C16—C19	120.9 (3)
C8—N3—Cd1^{iii}	124.6 (3)	C18—C17—C16	119.3 (4)
C18—N4—C14	118.0 (3)	C18—C17—H17A	120.4

C18—N4—Cd2	123.1 (3)	C16—C17—H17A	120.4
C14—N4—Cd2	117.7 (3)	N4—C18—C17	122.8 (4)
C20—N5—C21	106.6 (3)	N4—C18—H18A	118.6
C20—N5—C19	124.6 (3)	C17—C18—H18A	118.6
C21—N5—C19	128.3 (3)	N5—C19—C16	110.2 (3)
C20—N6—C26	106.4 (3)	N5—C19—H19A	109.6
C20—N6—Cd2^{iv}	124.7 (3)	C16—C19—H19A	109.6
C26—N6—Cd2^{iv}	128.9 (3)	N5—C19—H19B	109.6
N1—C1—C2	123.6 (4)	C16—C19—H19B	109.6
N1—C1—H1A	118.2	H19A—C19—H19B	108.1
C2—C1—H1A	118.2	N6—C20—N5	112.5 (4)
C1—C2—C3	119.5 (4)	N6—C20—H20A	123.7
C1—C2—H2A	120.3	N5—C20—H20A	123.7
C3—C2—H2A	120.3	C26—C21—C22	122.0 (4)
C2—C3—C4	117.3 (4)	C26—C21—N5	105.6 (3)
C2—C3—C6	124.3 (4)	C22—C21—N5	132.4 (4)
C4—C3—C6	118.4 (4)	C23—C22—C21	116.8 (4)
C5—C4—C3	119.3 (4)	C23—C22—H22A	121.6
C5—C4—H4A	120.4	C21—C22—H22A	121.6
C3—C4—H4A	120.4	C22—C23—C24	121.0 (4)
N1—C5—C4	123.1 (4)	C22—C23—H23A	119.5
N1—C5—H5A	118.4	C24—C23—H23A	119.5
C4—C5—H5A	118.4	C25—C24—C23	122.3 (4)
N2—C6—C3	115.0 (3)	C25—C24—H24A	118.8
N2—C6—H6A	108.5	C23—C24—H24A	118.8
C3—C6—H6A	108.5	C24—C25—C26	117.2 (4)
N2—C6—H6B	108.5	C24—C25—H25A	121.4
C3—C6—H6B	108.5	C26—C25—H25A	121.4
H6A—C6—H6B	107.5	C21—C26—C25	120.5 (4)
N3—C7—N2	114.2 (3)	C21—C26—N6	108.9 (3)
N3—C7—H7A	122.9	C25—C26—N6	130.6 (4)
N2—C7—H7A	122.9	O1—C27—H27A	109.5
N3—C8—C9	130.7 (4)	O1—C27—H27B	109.5
N3—C8—C13	109.8 (4)	H27A—C27—H27B	109.5
C9—C8—C13	119.5 (4)	O1—C27—H27C	109.5
C12—C13—C8	123.0 (4)	H27A—C27—H27C	109.5
C12—C13—N2	132.1 (4)	H27B—C27—H27C	109.5
C8—C13—N2	105.0 (3)	C27—O1—H1	109.5
C11—C12—C13	116.0 (4)		

N3^{i}—Cd1—N1—C1	92.6 (3)	N2—C13—C12—C11	179.2 (4)
I2—Cd1—N1—C1	−155.8 (3)	C13—C12—C11—C10	−0.8 (6)
I1—Cd1—N1—C1	−15.2 (3)	C12—C11—C10—C9	2.3 (6)
N3^{i}—Cd1—N1—C5	−94.8 (3)	C11—C10—C9—C8	−1.6 (6)
I2—Cd1—N1—C5	16.8 (3)	N3—C8—C9—C10	179.5 (4)
I1—Cd1—N1—C5	157.4 (3)	C13—C8—C9—C10	−0.4 (6)
N6^{ii}—Cd2—N4—C18	107.4 (3)	C18—N4—C14—C15	0.2 (6)
I3—Cd2—N4—C18	−141.9 (3)	Cd2—N4—C14—C15	−167.5 (3)

I4—Cd2—N4—C18	−6.1 (3)	N4—C14—C15—C16	1.1 (6)
N6^{ii}—Cd2—N4—C14	−85.6 (3)	C14—C15—C16—C17	−2.3 (6)
I3—Cd2—N4—C14	25.1 (3)	C14—C15—C16—C19	178.2 (4)
I4—Cd2—N4—C14	160.9 (3)	C15—C16—C17—C18	2.1 (6)
C5—N1—C1—C2	−1.2 (6)	C19—C16—C17—C18	−178.4 (3)
Cd1—N1—C1—C2	171.9 (3)	C14—N4—C18—C17	−0.4 (6)
N1—C1—C2—C3	3.5 (6)	Cd2—N4—C18—C17	166.6 (3)
C1—C2—C3—C4	−3.7 (6)	C16—C17—C18—N4	−0.8 (6)
C1—C2—C3—C6	173.8 (4)	C20—N5—C19—C16	88.7 (5)
C2—C3—C4—C5	1.9 (6)	C21—N5—C19—C16	−83.1 (4)
C6—C3—C4—C5	−175.7 (4)	C15—C16—C19—N5	59.9 (5)
C1—N1—C5—C4	−0.8 (6)	C17—C16—C19—N5	−119.7 (4)
Cd1—N1—C5—C4	−173.4 (3)	C26—N6—C20—N5	0.2 (4)
C3—C4—C5—N1	0.3 (6)	Cd2^{iv}—N6—C20—N5	179.3 (2)
C7—N2—C6—C3	121.7 (4)	C21—N5—C20—N6	−0.1 (5)
C13—N2—C6—C3	−61.8 (5)	C19—N5—C20—N6	−173.4 (3)
C2—C3—C6—N2	−0.4 (6)	C20—N5—C21—C26	0.0 (4)
C4—C3—C6—N2	177.1 (3)	C19—N5—C21—C26	172.9 (3)
C8—N3—C7—N2	−0.3 (4)	C20—N5—C21—C22	−179.4 (4)
Cd1^{iii}—N3—C7—N2	−174.1 (2)	C19—N5—C21—C22	−6.5 (7)
C13—N2—C7—N3	1.3 (4)	C26—C21—C22—C23	−1.6 (6)
C6—N2—C7—N3	178.3 (3)	N5—C21—C22—C23	177.7 (4)
C7—N3—C8—C9	179.2 (4)	C21—C22—C23—C24	0.2 (6)
Cd1^{iii}—N3—C8—C9	−6.6 (6)	C22—C23—C24—C25	1.5 (7)
C7—N3—C8—C13	−0.9 (4)	C23—C24—C25—C26	−1.8 (6)
Cd1^{iii}—N3—C8—C13	173.3 (2)	C22—C21—C26—C25	1.3 (6)
N3—C8—C13—C12	−178.0 (3)	N5—C21—C26—C25	−178.1 (3)
C9—C8—C13—C12	1.9 (6)	C22—C21—C26—N6	179.6 (4)
N3—C8—C13—N2	1.6 (4)	N5—C21—C26—N6	0.2 (4)
C9—C8—C13—N2	−178.4 (3)	C24—C25—C26—C21	0.4 (6)
C7—N2—C13—C12	177.9 (4)	C24—C25—C26—N6	−177.5 (4)
C6—N2—C13—C12	0.8 (6)	C20—N6—C26—C21	−0.2 (4)
C7—N2—C13—C8	−1.7 (4)	Cd2^{iv}—N6—C26—C21	−179.2 (3)
C6—N2—C13—C8	−178.8 (3)	C20—N6—C26—C25	177.8 (4)
C8—C13—C12—C11	−1.2 (6)	Cd2^{iv}—N6—C26—C25	−1.2 (6)

Symmetry codes: (i) x, $-y+3/2$, $z+1/2$; (ii) $-x+1$, $y-1/2$, $-z+3/2$; (iii) x, $-y+3/2$, $z-1/2$; (iv) $-x+1$, $y+1/2$, $-z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···I2^{v}	0.82	2.88	3.647 (5)	155

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