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Dibromido{*N*′-[1-(pyridin-2-yl)ethylidene]picolinohydrazide-κ^2N',O}cadmium

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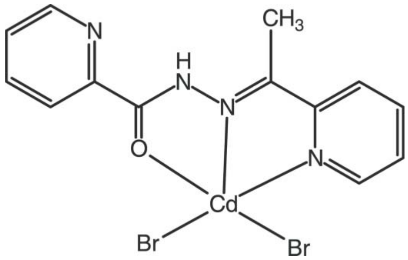
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.062; data-to-parameter ratio = 19.9.

The title compound, $[CdBr_2(C_{13}H_{12}N_4O)]$, was obtained from the reaction of $Cd(NO_3)_2\cdot4H_2O$ with methyl(pyridin-2-yl)methanone picolinoylhydrazone and sodium bromide. The Cd^{2+} cation is ligated by one O atom and two N atoms of the tridentate ligand and two bromide anions, forming a Br_2CdN_2O polyhedron with a distorted trigonal–bipyramidal coordination geometry. In the crystal, non-classical C—H$\cdots$Br hydrogen bonds are observed. In addition, π–π stacking interactions [centroid–centroid distance = 3.7455 (19) Å] contribute to the stabilization of the crystal structure.

Related literature

For related complexes with similar tridentate ligands, see: Kasuga *et al.* (2001); Chen *et al.* (2005); Datta *et al.* (2011).



Experimental

Crystal data

$[CdBr_2(C_{13}H_{12}N_4O)]$
M_r = 512.48
Monoclinic, $P2_1/n$
a = 8.1336 (3) Å
b = 13.6111 (5) Å
c = 14.6102 (5) Å
β = 90.550 (1)°
V = 1617.38 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.29 mm^{-1}
T = 296 K
0.32 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.267, T_{max} = 0.365
15317 measured reflections
3874 independent reflections
2859 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.062
S = 1.02
3874 reflections
195 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7$C\cdots$Br2^{i}	0.96	2.91	3.810 (4)	157

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2176).

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supplementary materials

Acta Cryst. (2012). E**68**, m842   [doi:10.1107/S1600536812023185]

Dibromido{*N′*-[1-(pyridin-2-yl)ethylidene]picolinohydrazide-κ^2*N′*,*O*}cadmium

Mehmet Akkurt, Ali Akbar Khandar, Muhammad Nawaz Tahir, Seyed Abolfazl Hosseini Yazdi and Farhad Akbari Afkhami

Comment

Schiff base complexes have attracted much attention due to their interesting structures and wide potential applications. Recently, the relative unsymmetrical tridentate Schiff base ligands and their hydrogenated derivatives have been introduced into the coordination chemistry to assemble polymers with beautiful molecular structures. Some organic N-donor ligands are often chosen to fabricate these various complexes. In this connection, some complexes with similar tridentate ligands have been studied (Kasuga *et al.*, 2001; Chen *et al.*, 2005; Datta *et al.*, 2011). Herein, we report the structure of a new cadmium complex based on a pyridine based tridentate Schiff base ligand.

The molecular structure of title compound is shown in Fig. 1. The Cd ion is five coordinated forming a distorted trigonal-bipyramidal coordination sphere, in which three positions are occupied by two N atoms and one O atom from the tridentate Schiff base ligand, and two positions coming from two bromide ions. As can be seen in Fig. 1, all non-H atoms of the tridentate Schiff base ligand are nearly coplanar, with maximum deviations of -0.053 (4) Å for C7 and 0.049 (2) Å for N2.

Molecules are linked to each other, *via* weak C—H···Br intermolecular hydrogen bonds along the crystallographic *a* axis (Table 1, Fig. 2). In the crystal, weak π-π stacking interactions also contribute to the stabilization: [$Cg3\cdots Cg3(1 - x, -y, 1 - z)$ = 3.7455 (19) Å; where *Cg*3 is the centroid of the N1/C1–C5 ring].

Experimental

The potentially tridenatate ligand methyl-2-pyridyl ketone picolinoyl hydrazone was obtained by condensation of methyl-2-pyridyl ketone and picolinic acid hydrazide with the ratio 1:1 in methanol. The title compound $C_{13}H_{12}Br_2CdN_4O$ has been synthesized by the reaction of methanolic solution of the ligand and $Cd(NO_3)_2.4H_2O$ in the presence of excess amount of NaBr. The ligand (1 mmol, 0.240 g) and cadmium nitrate (1 mmol, 279 g) were placed in main arm of a branched tube; sodium bromide (2 mmol, 0.206 g) was added to the mixture too. Methanol was carefully added to fill the arms. The tube was sealed and the ligand-containing arm was immersed in an oil bath at 333 K while the branched arm was kept at ambient temperature. After five days, suitable single crystals, were deposited in the cooler arm which were isolated, filtered off, washed with acetone and ether and air dried.

Refinement

H atoms bonded to C atoms were positioned geometrically and treated as riding with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H, and C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H. The amine H atom was located in difference Fourier map and refined freely [N—H = 0.86 (2) Å].

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

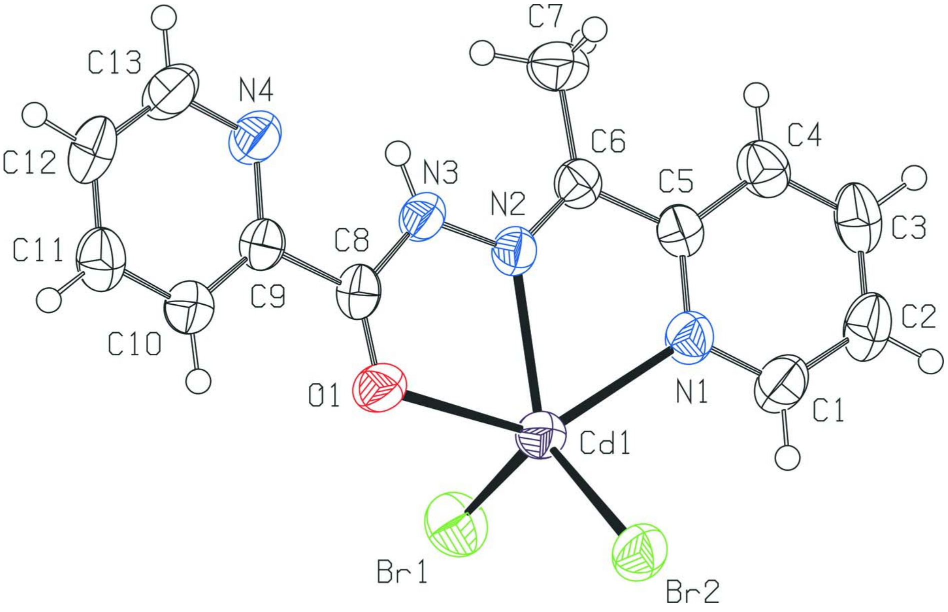

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

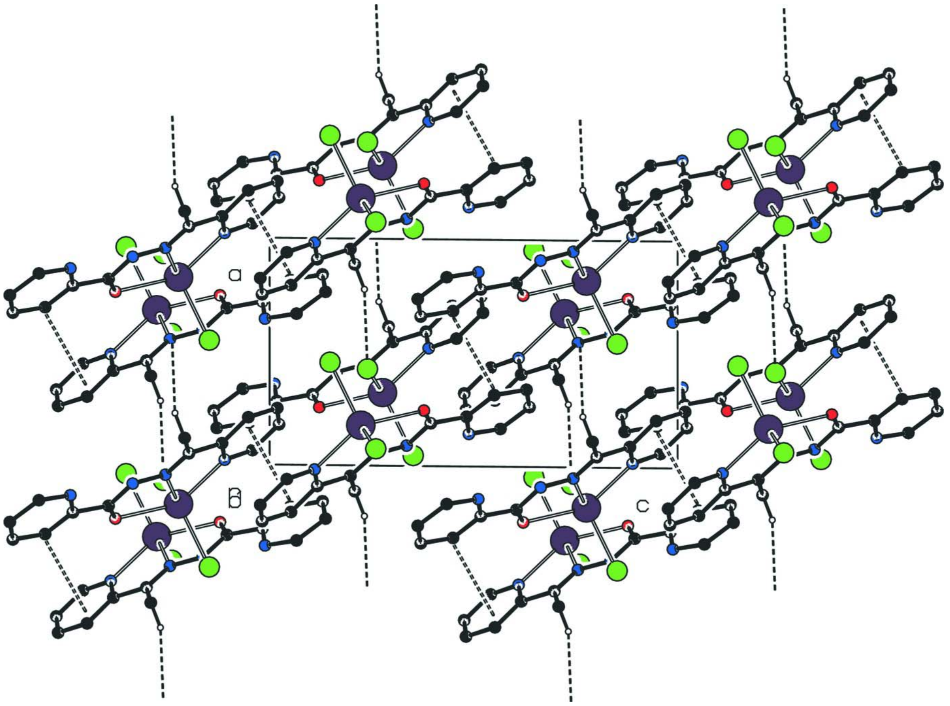

Figure 2

View of the intermolecular C—H···Br hydrogen bonds and π-π stacking interactions of the title compound. H atoms not involved in hydrogen bonding are omitted.

Dibromido{*N*′-[1-(pyridin-2-yl)ethylidene]picolinohydrazide- κ^2*N*′,*O*}cadmium

Crystal data

$[CdBr_2(C_{13}H_{12}N_4O)]$
$M_r = 512.48$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.1336\ (3)$ Å
$b = 13.6111\ (5)$ Å
$c = 14.6102\ (5)$ Å
$\beta = 90.550\ (1)°$
$V = 1617.38\ (10)$ Å^3
$Z = 4$

$F(000) = 976$
$D_x = 2.105$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 545 reflections
$\theta = 4.2–18.3°$
$\mu = 6.29$ mm^{-1}
$T = 296$ K
Prism, colourless
0.32 × 0.18 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.267$, $T_{max} = 0.365$

15317 measured reflections
3874 independent reflections
2859 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 28.1°$, $\theta_{min} = 2.9°$
$h = -10\rightarrow10$
$k = -17\rightarrow18$
$l = -19\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.062$
$S = 1.02$
3874 reflections
195 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.5132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.32238 (3)	0.16938 (2)	0.27655 (2)	0.0429 (1)
Br1	0.04606 (5)	0.15378 (3)	0.35202 (3)	0.0626 (1)
Br2	0.42596 (5)	0.34049 (2)	0.23982 (3)	0.0550 (1)
O1	0.2555 (3)	0.10824 (15)	0.12175 (14)	0.0493 (8)
N1	0.5195 (3)	0.12698 (18)	0.38976 (17)	0.0438 (9)
N2	0.4511 (3)	0.02135 (16)	0.24438 (15)	0.0370 (8)
N3	0.4106 (3)	−0.02318 (18)	0.16427 (17)	0.0401 (8)
N4	0.3565 (3)	−0.11450 (19)	0.01147 (18)	0.0495 (10)
C1	0.5632 (5)	0.1867 (2)	0.4579 (2)	0.0555 (11)
C2	0.6781 (5)	0.1618 (3)	0.5230 (2)	0.0585 (11)
C3	0.7498 (4)	0.0712 (3)	0.5186 (2)	0.0585 (14)
C4	0.7079 (4)	0.0090 (2)	0.4477 (2)	0.0487 (11)
C5	0.5925 (4)	0.0390 (2)	0.3832 (2)	0.0385 (9)
C6	0.5464 (3)	−0.0217 (2)	0.3021 (2)	0.0377 (9)
C7	0.6137 (5)	−0.1226 (2)	0.2915 (2)	0.0577 (11)
C8	0.3114 (4)	0.0268 (2)	0.1050 (2)	0.0392 (9)
C9	0.2810 (4)	−0.0274 (2)	0.01743 (19)	0.0381 (9)
C10	0.1844 (4)	0.0113 (2)	−0.0505 (2)	0.0473 (11)
C11	0.1592 (4)	−0.0425 (2)	−0.1296 (2)	0.0523 (11)
C12	0.2361 (5)	−0.1319 (2)	−0.1370 (2)	0.0543 (11)
C13	0.3333 (5)	−0.1652 (2)	−0.0658 (2)	0.0569 (13)
H1	0.51340	0.24800	0.46140	0.0660*
H2	0.70680	0.20560	0.56930	0.0700*
H3	0.82590	0.05170	0.56290	0.0700*
H3N	0.434 (4)	−0.0819 (15)	0.150 (2)	0.056 (10)*

H4	0.75670	−0.05260	0.44310	0.0580*
H7A	0.54530	−0.15920	0.24990	0.0860*
H7B	0.61610	−0.15480	0.34990	0.0860*
H7C	0.72320	−0.11890	0.26780	0.0860*
H10	0.13630	0.07280	−0.04360	0.0570*
H11	0.09200	−0.01880	−0.17650	0.0630*
H12	0.22280	−0.16960	−0.18970	0.0650*
H13	0.38510	−0.22580	−0.07180	0.0680*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0474 (1)	0.0383 (1)	0.0428 (1)	0.0045 (1)	−0.0051 (1)	−0.0016 (1)
Br1	0.0532 (2)	0.0726 (3)	0.0622 (2)	−0.0011 (2)	0.0063 (2)	0.0021 (2)
Br2	0.0638 (2)	0.0413 (2)	0.0598 (2)	−0.0049 (2)	−0.0091 (2)	0.0024 (2)
O1	0.0616 (15)	0.0432 (13)	0.0429 (12)	0.0105 (11)	−0.0085 (11)	−0.0083 (10)
N1	0.0503 (16)	0.0397 (14)	0.0412 (15)	−0.0023 (12)	−0.0086 (12)	0.0021 (11)
N2	0.0393 (14)	0.0367 (13)	0.0350 (14)	−0.0022 (11)	−0.0031 (11)	−0.0016 (10)
N3	0.0476 (15)	0.0354 (14)	0.0373 (14)	−0.0005 (12)	−0.0045 (11)	−0.0063 (11)
N4	0.0654 (19)	0.0394 (15)	0.0436 (16)	0.0006 (13)	−0.0089 (13)	−0.0043 (12)
C1	0.075 (2)	0.0403 (18)	0.051 (2)	−0.0047 (17)	−0.0117 (18)	−0.0030 (15)
C2	0.071 (2)	0.061 (2)	0.0433 (19)	−0.0144 (19)	−0.0141 (17)	−0.0057 (16)
C3	0.056 (2)	0.073 (3)	0.046 (2)	−0.0134 (18)	−0.0175 (17)	0.0083 (17)
C4	0.0471 (19)	0.0505 (19)	0.0483 (19)	−0.0019 (15)	−0.0065 (15)	0.0107 (15)
C5	0.0371 (16)	0.0401 (16)	0.0381 (16)	−0.0056 (13)	−0.0025 (13)	0.0074 (13)
C6	0.0359 (16)	0.0361 (16)	0.0411 (17)	−0.0045 (13)	0.0005 (13)	0.0033 (13)
C7	0.065 (2)	0.0458 (19)	0.062 (2)	0.0137 (17)	−0.0072 (18)	−0.0003 (17)
C8	0.0396 (16)	0.0418 (17)	0.0362 (16)	−0.0092 (14)	−0.0016 (13)	0.0004 (13)
C9	0.0384 (16)	0.0383 (16)	0.0376 (16)	−0.0058 (13)	0.0000 (13)	−0.0005 (12)
C10	0.0495 (19)	0.0458 (18)	0.0464 (19)	0.0008 (15)	−0.0065 (15)	−0.0043 (15)
C11	0.056 (2)	0.057 (2)	0.0437 (19)	−0.0102 (17)	−0.0101 (16)	0.0044 (15)
C12	0.069 (2)	0.053 (2)	0.0408 (19)	−0.0194 (18)	−0.0046 (17)	−0.0082 (15)
C13	0.075 (3)	0.0397 (18)	0.056 (2)	−0.0021 (17)	−0.0054 (19)	−0.0107 (16)

Geometric parameters (Å, º)

Cd1—Br1	2.5218 (5)	C5—C6	1.490 (4)
Cd1—Br2	2.5359 (4)	C6—C7	1.487 (4)
Cd1—O1	2.466 (2)	C8—C9	1.495 (4)
Cd1—N1	2.364 (2)	C9—C10	1.366 (4)
Cd1—N2	2.321 (2)	C10—C11	1.382 (4)
O1—C8	1.224 (4)	C11—C12	1.373 (4)
N1—C1	1.331 (4)	C12—C13	1.377 (5)
N1—C5	1.341 (4)	C1—H1	0.9300
N2—N3	1.356 (3)	C2—H2	0.9300
N2—C6	1.282 (4)	C3—H3	0.9300
N3—C8	1.360 (4)	C4—H4	0.9300
N4—C9	1.338 (4)	C7—H7A	0.9600
N4—C13	1.335 (4)	C7—H7B	0.9600
N3—H3N	0.85 (2)	C7—H7C	0.9600

C1—C2	1.370 (5)	C10—H10	0.9300
C2—C3	1.366 (6)	C11—H11	0.9300
C3—C4	1.378 (4)	C12—H12	0.9300
C4—C5	1.385 (4)	C13—H13	0.9300

Br1—Cd1—Br2	117.98 (2)	O1—C8—N3	123.0 (3)
Br1—Cd1—O1	100.54 (6)	O1—C8—C9	124.0 (3)
Br1—Cd1—N1	105.95 (6)	C8—C9—C10	121.4 (3)
Br1—Cd1—N2	114.91 (6)	N4—C9—C8	114.9 (3)
Br2—Cd1—O1	100.76 (5)	N4—C9—C10	123.8 (3)
Br2—Cd1—N1	98.50 (6)	C9—C10—C11	118.9 (3)
Br2—Cd1—N2	127.09 (6)	C10—C11—C12	118.1 (3)
O1—Cd1—N1	134.55 (8)	C11—C12—C13	119.4 (3)
O1—Cd1—N2	67.49 (8)	N4—C13—C12	123.0 (3)
N1—Cd1—N2	68.01 (8)	N1—C1—H1	118.00
Cd1—O1—C8	114.21 (19)	C2—C1—H1	119.00
Cd1—N1—C1	123.3 (2)	C1—C2—H2	121.00
Cd1—N1—C5	117.77 (19)	C3—C2—H2	121.00
C1—N1—C5	118.9 (3)	C2—C3—H3	120.00
Cd1—N2—N3	117.17 (17)	C4—C3—H3	120.00
Cd1—N2—C6	122.33 (18)	C3—C4—H4	120.00
N3—N2—C6	120.3 (2)	C5—C4—H4	120.00
N2—N3—C8	117.6 (2)	C6—C7—H7A	109.00
C9—N4—C13	116.9 (3)	C6—C7—H7B	109.00
C8—N3—H3N	117 (2)	C6—C7—H7C	109.00
N2—N3—H3N	126 (2)	H7A—C7—H7B	109.00
N1—C1—C2	123.0 (3)	H7A—C7—H7C	109.00
C1—C2—C3	118.7 (3)	H7B—C7—H7C	109.00
C2—C3—C4	119.2 (3)	C9—C10—H10	121.00
C3—C4—C5	119.4 (3)	C11—C10—H10	121.00
N1—C5—C4	120.8 (3)	C10—C11—H11	121.00
C4—C5—C6	122.8 (3)	C12—C11—H11	121.00
N1—C5—C6	116.4 (3)	C11—C12—H12	120.00
N2—C6—C7	125.1 (3)	C13—C12—H12	120.00
C5—C6—C7	120.3 (2)	N4—C13—H13	119.00
N2—C6—C5	114.6 (2)	C12—C13—H13	119.00
N3—C8—C9	113.0 (2)		

Br1—Cd1—O1—C8	−107.6 (2)	Cd1—N2—C6—C7	170.9 (2)
Br2—Cd1—O1—C8	131.0 (2)	Cd1—N2—N3—C8	6.6 (3)
N1—Cd1—O1—C8	17.6 (3)	Cd1—N2—C6—C5	−11.0 (3)
N2—Cd1—O1—C8	5.2 (2)	N3—N2—C6—C7	−3.4 (4)
Br1—Cd1—N1—C1	−76.1 (3)	N3—N2—C6—C5	174.8 (2)
Br2—Cd1—N1—C1	46.4 (3)	N2—N3—C8—O1	−1.5 (4)
O1—Cd1—N1—C1	160.7 (2)	N2—N3—C8—C9	177.5 (2)
N2—Cd1—N1—C1	173.0 (3)	C9—N4—C13—C12	−0.5 (5)
Br1—Cd1—N1—C5	105.4 (2)	C13—N4—C9—C8	−179.7 (3)
Br2—Cd1—N1—C5	−132.2 (2)	C13—N4—C9—C10	−0.4 (5)
O1—Cd1—N1—C5	−17.9 (3)	N1—C1—C2—C3	−0.8 (6)

N2—Cd1—N1—C5	−5.6 (2)	C1—C2—C3—C4	1.8 (5)
Br1—Cd1—N2—N3	85.55 (18)	C2—C3—C4—C5	−0.9 (5)
Br2—Cd1—N2—N3	−92.50 (19)	C3—C4—C5—N1	−1.0 (5)
O1—Cd1—N2—N3	−5.94 (17)	C3—C4—C5—C6	177.0 (3)
N1—Cd1—N2—N3	−176.5 (2)	N1—C5—C6—N2	5.2 (4)
Br1—Cd1—N2—C6	−88.8 (2)	C4—C5—C6—C7	5.3 (4)
Br2—Cd1—N2—C6	93.1 (2)	C4—C5—C6—N2	−172.9 (3)
O1—Cd1—N2—C6	179.7 (2)	N1—C5—C6—C7	−176.6 (3)
N1—Cd1—N2—C6	9.2 (2)	O1—C8—C9—N4	178.4 (3)
Cd1—O1—C8—C9	177.1 (2)	N3—C8—C9—C10	−179.9 (3)
Cd1—O1—C8—N3	−4.0 (4)	O1—C8—C9—C10	−1.0 (5)
Cd1—N1—C5—C6	2.6 (3)	N3—C8—C9—N4	−0.6 (4)
Cd1—N1—C1—C2	−179.7 (3)	N4—C9—C10—C11	1.4 (5)
C1—N1—C5—C4	2.0 (4)	C8—C9—C10—C11	−179.3 (3)
C1—N1—C5—C6	−176.1 (3)	C9—C10—C11—C12	−1.5 (5)
C5—N1—C1—C2	−1.1 (5)	C10—C11—C12—C13	0.7 (5)
Cd1—N1—C5—C4	−179.3 (2)	C11—C12—C13—N4	0.3 (6)
C6—N2—N3—C8	−178.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*C*···Br2^{i}	0.96	2.91	3.810 (4)	157

Symmetry code: (i) $-x+3/2, y-1/2, -z+1/2$.