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Dibromidobis(2-methyl-1*H*-benzimidazole-κN^3)cadmium

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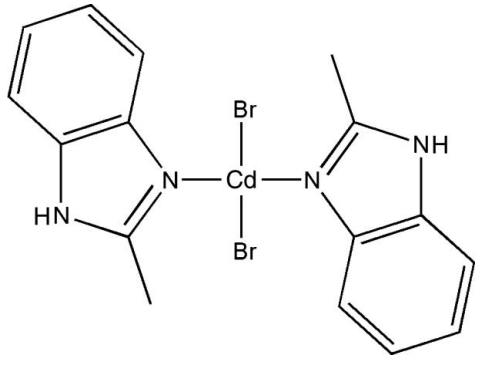
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.077; data-to-parameter ratio = 17.1.

In the title compound, $[CdBr_2(C_8H_8N_2)_2]$, the Cd^{II} atom has a distorted tetrahedral coordination formed by the two imino N atoms of two 2-methylbenzimidazole ligands and two terminal bromide ligands. The Cd^{II} atom is slightly out of the benzimidazole planes by 0.320 (3) and 0.210 (3) Å. The dihedral angle between the benzimidazole planes is 71.6 (2)°. In the crystal, molecules are linked by N—H···Br hydrogen bonds into puckered layers parallel to (001).

Related literature

For background to benzimidazole, see: Roderick *et al.* (1972). For related crystal structures, see: Barros-García *et al.* (2005); Wang *et al.* (2010); Yang *et al.* (2011).



Experimental

Crystal data

$[CdBr_2(C_8H_8N_2)_2]$ M_r = 536.54
Monoclinic, $P2_1/c$
a = 10.007 (9) Å
b = 14.747 (12) Å
c = 12.399 (11) Å
β = 93.088 (14)°
V = 1827 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.57 mm^{-1}
T = 296 K
0.22 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.374, T_{max} = 0.469
9698 measured reflections
3585 independent reflections
2748 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.077
S = 1.00
3585 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···Br1^{i}	0.86	2.88	3.495 (4)	130
N4—H4···Br2^{ii}	0.86	2.77	3.563 (4)	155

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); 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: KQ2008).

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supplementary materials

Acta Cryst. (2013). E**69**, m536 [doi:10.1107/S1600536813024549]

Dibromidobis(2-methyl-1*H*-benzimidazole-κN^3)cadmium

Bao-Cheng Liu, Yan-Ling Jin and Fa-Qian Liu

1. Comment

Benzimidazole and its derivatives have attracted interest because their biological activities as well as their abilities to bind different metal ions (Roderick *et al.*, 1972). In this paper, we describe the synthesis and structure of dibromo-bis(2-methylbenzimidazole)-cadmium(II).

In the title compound, $C_{16}H_{16}CdBr_2N_4$, the cadmium atom has a distorted tetrahedral coordination formed by the two imino-nitrogen atoms of two 2-methyl-benzimidazole ligands and two terminal bromide ligands (Figure 1). The similar geometry was previously found in the related compounds – $Cd(Cl)_2$(*N*-(5,6-dihydro-4*H*- 1,3-thiazin-2-yl)-2-amino-benzimidazole)$_2$ (Barros-García *et al.*, 2005), $Cd(Cl)_2$(2-(2-furyl)-1-(2-furylmethyl)-1*H*-benzimidazole)$_2$ (Wang *et al.*, 2010), and $Cd(I)_2$(2-(2-furyl)-1-(2-furylmethyl)- 1*H*-enzimidazole)$_2$ (Yang *et al.*, 2011). The cadmium atom is slightly out of the two benzimidazole planes by 0.320 (3) and 0.210 (3) Å, respectively. The dihedral angle between the two benzimidazole planes is 71.6 (2)°. The mean values of Cd—Br and Cd—N bond lengths are 2.562 (2) and 2.251 (3) Å, respectively. The N—Cd—Br bond angles range from 105.40 (10) to 117.76 (9)°.

In the crystal, the molecules of the title compound are linked by intermolecular N2—H2···Br1^{i} and N4—H4···Br2^{ii} hydrogen bonds (Table 1) into puckered layers parallel to (001) (Figure 2). Symmetry codes: (i) –*x*+1, *y*–1/2, –*z*+3/2; (ii) –*x*, *y*–1/2, –*z*+3/2.

2. Experimental

The ligand 2-methyl-benzimidazole (0.02 mmol) in ethanol (10 mL) was added dropwise to a ethanol (10 mL) of $CdBr_2$ (0.01 mmol). The resulting solution was allowed to stand at room temperature. After one week colorless crystals with good quality were obtained from the filtrate and dried in air. Analysis, calculated for $C_{16}H_{16}Br_2CdN_4$: C 35.82, H 3.01, N 10.44%; Found: C 35.68, H 3.02, N 10.47%.

3. Refinement

All hydrogen atoms were placed in calculated positions with N—H = 0.86 Å and C—H = 0.93 (aryl-H) and 0.96 (methyl-H) Å and refined in the riding model with fixed isotropic displacement parameters [U_{iso}(H) = 1.2U_{eq}(N or C)].

Computing details

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO* (Rigaku, 2004); data reduction: *RAPID-AUTO* (Rigaku, 2004); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

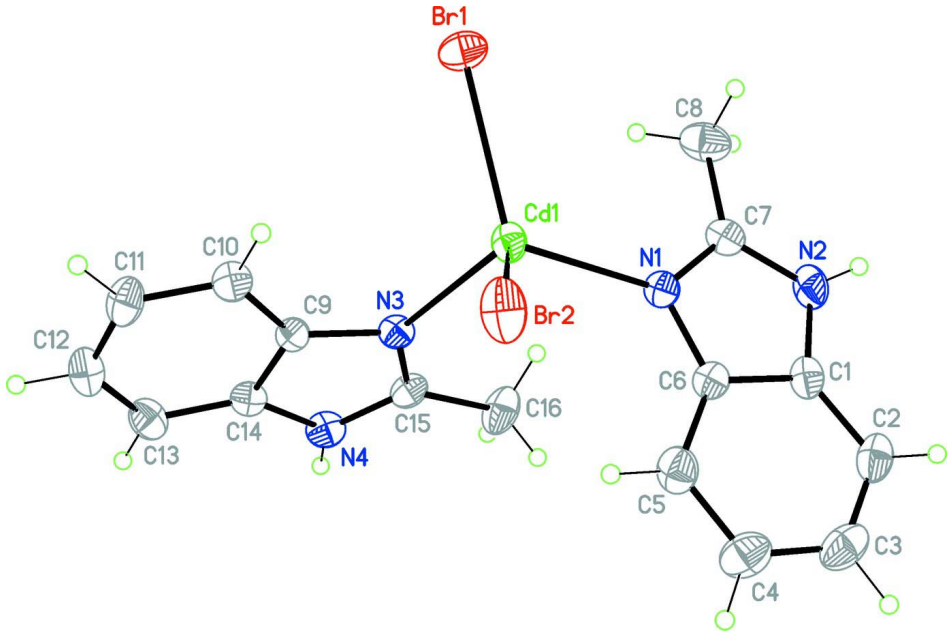

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are shown at the 40% probability level. H atoms are presented as small spheres of arbitrary radius.

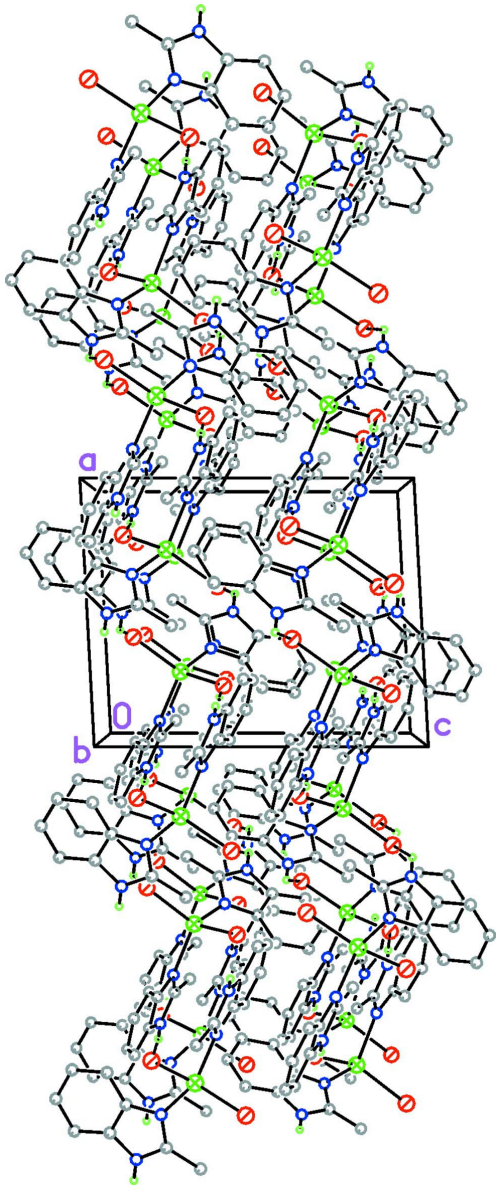

Figure 2

Crystal packing of the title compound along the *b* axis demonstrating the puckered layers parallel to (001). Dashed lines indicate the intermolecular hydrogen bonds.

Dibromidobis(2-methyl-1*H*-benzimidazole-κN^3)cadmium

Crystal data

$[CdBr_2(C_8H_8N_2)_2]$
$M_r = 536.54$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.007$ (9) Å
$b = 14.747$ (12) Å
$c = 12.399$ (11) Å
$\beta = 93.088$ (14)°
$V = 1827$ (3) Å^3
$Z = 4$
$F(000) = 1032$
$D_x = 1.951$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3275 reflections
$\theta = 2.5$–26.6°
$\mu = 5.57$ mm^{-1}

T = 296 K
Block, colorless

0.22 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.374, T_{max} = 0.469
9698 measured reflections

3585 independent reflections
2748 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°, θ_{min} = 2.0°
h = −12→10
k = −18→14
l = −15→14
13 standard reflections every 0 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.077
S = 1.00
3585 reflections
210 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
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −1.02 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}
N1	0.3592 (3)	0.96335 (19)	0.8577 (2)	0.0362 (7)
N2	0.5028 (4)	0.8661 (2)	0.9341 (3)	0.0485 (9)
H2	0.5712	0.8311	0.9428	0.058*
N3	0.0723 (3)	1.01679 (18)	0.6820 (2)	0.0339 (7)
N4	−0.1049 (3)	0.93220 (19)	0.6357 (2)	0.0417 (8)
H4	−0.1554	0.8851	0.6290	0.050*
Br1	0.40130 (5)	1.14156 (3)	0.60773 (4)	0.06071 (16)
Br2	0.20546 (5)	1.20099 (3)	0.88850 (4)	0.06367 (17)
C1	0.4087 (4)	0.8806 (2)	1.0086 (3)	0.0409 (9)
C2	0.3939 (5)	0.8457 (3)	1.1109 (3)	0.0531 (12)
H2A	0.4561	0.8060	1.1434	0.064*
C3	0.2816 (6)	0.8730 (3)	1.1622 (4)	0.0626 (14)
H3	0.2681	0.8511	1.2311	0.075*
C4	0.1873 (6)	0.9326 (3)	1.1139 (4)	0.0633 (13)

H4A	0.1119	0.9482	1.1505	0.076*
C5	0.2045 (5)	0.9687 (3)	1.0127 (3)	0.0535 (11)
H5	0.1432	1.0094	0.9812	0.064*
C6	0.3175 (4)	0.9417 (2)	0.9597 (3)	0.0368 (9)
C7	0.4708 (4)	0.9156 (2)	0.8454 (3)	0.0408 (9)
C8	0.5489 (5)	0.9139 (3)	0.7478 (4)	0.0620 (13)
H8A	0.4935	0.9338	0.6867	0.093*
H8B	0.5793	0.8532	0.7355	0.093*
H8C	0.6246	0.9536	0.7578	0.093*
C9	−0.0236 (4)	1.0707 (2)	0.6250 (3)	0.0332 (8)
C10	−0.0180 (4)	1.1618 (2)	0.5961 (3)	0.0420 (9)
H10	0.0571	1.1972	0.6131	0.050*
C11	−0.1303 (5)	1.1972 (3)	0.5406 (3)	0.0502 (11)
H11	−0.1297	1.2575	0.5187	0.060*
C12	−0.2441 (5)	1.1449 (3)	0.5168 (3)	0.0531 (11)
H12	−0.3184	1.1720	0.4820	0.064*
C13	−0.2499 (4)	1.0548 (3)	0.5431 (3)	0.0482 (10)
H13	−0.3255	1.0199	0.5259	0.058*
C14	−0.1372 (4)	1.0184 (2)	0.5966 (3)	0.0364 (9)
C15	0.0180 (4)	0.9343 (2)	0.6856 (3)	0.0386 (9)
C16	0.0818 (5)	0.8531 (2)	0.7384 (3)	0.0577 (13)
H16A	0.1749	0.8514	0.7233	0.087*
H16B	0.0384	0.7992	0.7108	0.087*
H16C	0.0733	0.8566	0.8150	0.087*
Cd1	0.26490 (3)	1.074421 (18)	0.75481 (2)	0.03930 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.039 (2)	0.0255 (15)	0.0436 (18)	0.0043 (14)	0.0033 (15)	0.0002 (14)
N2	0.044 (2)	0.0340 (18)	0.066 (2)	0.0133 (15)	−0.0060 (18)	0.0078 (17)
N3	0.0365 (18)	0.0242 (15)	0.0410 (16)	−0.0068 (13)	0.0015 (14)	−0.0021 (13)
N4	0.048 (2)	0.0289 (17)	0.0482 (19)	−0.0128 (14)	0.0016 (16)	−0.0055 (14)
Br1	0.0653 (3)	0.0460 (3)	0.0713 (3)	−0.0150 (2)	0.0077 (2)	0.0149 (2)
Br2	0.0746 (4)	0.0398 (3)	0.0745 (3)	0.0205 (2)	−0.0163 (3)	−0.0179 (2)
C1	0.044 (2)	0.027 (2)	0.050 (2)	−0.0007 (17)	−0.010 (2)	0.0000 (18)
C2	0.066 (3)	0.039 (2)	0.053 (3)	−0.008 (2)	−0.017 (2)	0.006 (2)
C3	0.089 (4)	0.058 (3)	0.041 (2)	−0.018 (3)	0.003 (3)	−0.003 (2)
C4	0.082 (4)	0.057 (3)	0.052 (3)	0.005 (3)	0.016 (3)	−0.005 (2)
C5	0.058 (3)	0.049 (3)	0.053 (3)	0.016 (2)	0.002 (2)	−0.003 (2)
C6	0.043 (2)	0.0256 (19)	0.041 (2)	−0.0001 (16)	0.0017 (18)	−0.0006 (16)
C7	0.039 (2)	0.030 (2)	0.053 (2)	0.0008 (17)	0.0057 (19)	−0.0037 (18)
C8	0.057 (3)	0.050 (3)	0.081 (3)	0.006 (2)	0.027 (3)	−0.005 (2)
C9	0.037 (2)	0.030 (2)	0.0328 (19)	0.0039 (16)	0.0046 (16)	−0.0025 (16)
C10	0.046 (3)	0.033 (2)	0.048 (2)	−0.0044 (18)	0.0004 (19)	−0.0034 (18)
C11	0.068 (3)	0.029 (2)	0.053 (2)	0.013 (2)	−0.003 (2)	−0.0004 (19)
C12	0.051 (3)	0.054 (3)	0.053 (3)	0.013 (2)	−0.010 (2)	−0.006 (2)
C13	0.041 (3)	0.053 (3)	0.050 (2)	−0.004 (2)	−0.005 (2)	−0.011 (2)
C14	0.041 (2)	0.035 (2)	0.0341 (19)	−0.0006 (17)	0.0046 (17)	−0.0080 (16)
C15	0.051 (3)	0.028 (2)	0.038 (2)	−0.0037 (17)	0.0054 (19)	0.0007 (16)

C16	0.082 (4)	0.030 (2)	0.059 (3)	−0.008 (2)	−0.014 (2)	0.011 (2)
Cd1	0.04113 (19)	0.02686 (16)	0.04918 (18)	0.00061 (12)	−0.00430 (13)	0.00266 (12)

Geometric parameters (Å, º)

N1—C7	1.336 (5)	C4—H4A	0.9300
N1—C6	1.390 (5)	C5—C6	1.396 (6)
N1—Cd1	2.252 (3)	C5—H5	0.9300
N2—C7	1.345 (5)	C7—C8	1.475 (6)
N2—C1	1.370 (5)	C8—H8A	0.9600
N2—H2	0.8600	C8—H8B	0.9600
N3—C15	1.334 (4)	C8—H8C	0.9600
N3—C9	1.407 (5)	C9—C10	1.393 (5)
N3—Cd1	2.250 (3)	C9—C14	1.403 (5)
N4—C15	1.347 (5)	C10—C11	1.387 (6)
N4—C14	1.392 (5)	C10—H10	0.9300
N4—H4	0.8600	C11—C12	1.394 (6)
Br1—Cd1	2.5372 (15)	C11—H11	0.9300
Br2—Cd1	2.5869 (15)	C12—C13	1.370 (6)
C1—C2	1.385 (6)	C12—H12	0.9300
C1—C6	1.398 (5)	C13—C14	1.386 (6)
C2—C3	1.381 (7)	C13—H13	0.9300
C2—H2A	0.9300	C15—C16	1.492 (5)
C3—C4	1.401 (7)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C5	1.381 (6)	C16—H16C	0.9600
C7—N1—C6	106.1 (3)	C7—C8—H8C	109.5
C7—N1—Cd1	130.2 (3)	H8A—C8—H8C	109.5
C6—N1—Cd1	123.1 (2)	H8B—C8—H8C	109.5
C7—N2—C1	109.0 (3)	C10—C9—C14	120.6 (4)
C7—N2—H2	125.5	C10—C9—N3	129.7 (4)
C1—N2—H2	125.5	C14—C9—N3	109.7 (3)
C15—N3—C9	105.3 (3)	C11—C10—C9	116.6 (4)
C15—N3—Cd1	132.3 (3)	C11—C10—H10	121.7
C9—N3—Cd1	122.3 (2)	C9—C10—H10	121.7
C15—N4—C14	109.1 (3)	C10—C11—C12	121.9 (4)
C15—N4—H4	125.4	C10—C11—H11	119.1
C14—N4—H4	125.4	C12—C11—H11	119.1
N2—C1—C2	132.2 (4)	C13—C12—C11	122.1 (4)
N2—C1—C6	105.3 (3)	C13—C12—H12	119.0
C2—C1—C6	122.5 (4)	C11—C12—H12	119.0
C3—C2—C1	116.3 (4)	C12—C13—C14	116.5 (4)
C3—C2—H2A	121.8	C12—C13—H13	121.8
C1—C2—H2A	121.8	C14—C13—H13	121.8
C2—C3—C4	122.2 (4)	C13—C14—N4	133.4 (4)
C2—C3—H3	118.9	C13—C14—C9	122.3 (4)
C4—C3—H3	118.9	N4—C14—C9	104.2 (3)
C5—C4—C3	121.0 (5)	N3—C15—N4	111.7 (3)
C5—C4—H4A	119.5	N3—C15—C16	125.5 (4)

C3—C4—H4A	119.5	N4—C15—C16	122.8 (3)
C4—C5—C6	117.5 (4)	C15—C16—H16A	109.5
C4—C5—H5	121.2	C15—C16—H16B	109.5
C6—C5—H5	121.2	H16A—C16—H16B	109.5
N1—C6—C5	130.8 (4)	C15—C16—H16C	109.5
N1—C6—C1	108.8 (3)	H16A—C16—H16C	109.5
C5—C6—C1	120.4 (4)	H16B—C16—H16C	109.5
N1—C7—N2	110.8 (3)	N3—Cd1—N1	106.04 (12)
N1—C7—C8	125.9 (4)	N3—Cd1—Br1	109.95 (9)
N2—C7—C8	123.3 (4)	N1—Cd1—Br1	117.77 (9)
C7—C8—H8A	109.5	N3—Cd1—Br2	107.95 (9)
C7—C8—H8B	109.5	N1—Cd1—Br2	105.40 (9)
H8A—C8—H8B	109.5	Br1—Cd1—Br2	109.28 (2)

C7—N2—C1—C2	178.9 (4)	C9—C10—C11—C12	1.2 (6)
C7—N2—C1—C6	0.1 (4)	C10—C11—C12—C13	−2.5 (7)
N2—C1—C2—C3	−177.2 (4)	C11—C12—C13—C14	1.1 (6)
C6—C1—C2—C3	1.3 (6)	C12—C13—C14—N4	−179.9 (4)
C1—C2—C3—C4	0.1 (7)	C12—C13—C14—C9	1.4 (6)
C2—C3—C4—C5	−1.5 (7)	C15—N4—C14—C13	−177.7 (4)
C3—C4—C5—C6	1.5 (7)	C15—N4—C14—C9	1.2 (4)
C7—N1—C6—C5	−177.1 (4)	C10—C9—C14—C13	−2.7 (6)
Cd1—N1—C6—C5	11.3 (6)	N3—C9—C14—C13	177.7 (3)
C7—N1—C6—C1	0.9 (4)	C10—C9—C14—N4	178.3 (3)
Cd1—N1—C6—C1	−170.7 (2)	N3—C9—C14—N4	−1.4 (4)
C4—C5—C6—N1	177.6 (4)	C9—N3—C15—N4	−0.2 (4)
C4—C5—C6—C1	−0.2 (6)	Cd1—N3—C15—N4	175.6 (2)
N2—C1—C6—N1	−0.6 (4)	C9—N3—C15—C16	−179.7 (4)
C2—C1—C6—N1	−179.5 (3)	Cd1—N3—C15—C16	−3.9 (6)
N2—C1—C6—C5	177.6 (4)	C14—N4—C15—N3	−0.6 (4)
C2—C1—C6—C5	−1.3 (6)	C14—N4—C15—C16	178.9 (4)
C6—N1—C7—N2	−0.9 (4)	C15—N3—Cd1—N1	−4.6 (3)
Cd1—N1—C7—N2	169.9 (2)	C9—N3—Cd1—N1	170.6 (2)
C6—N1—C7—C8	177.7 (4)	C15—N3—Cd1—Br1	123.7 (3)
Cd1—N1—C7—C8	−11.5 (6)	C9—N3—Cd1—Br1	−61.0 (3)
C1—N2—C7—N1	0.5 (4)	C15—N3—Cd1—Br2	−117.1 (3)
C1—N2—C7—C8	−178.1 (4)	C9—N3—Cd1—Br2	58.1 (3)
C15—N3—C9—C10	−178.6 (4)	C7—N1—Cd1—N3	112.4 (3)
Cd1—N3—C9—C10	5.1 (5)	C6—N1—Cd1—N3	−78.2 (3)
C15—N3—C9—C14	1.0 (4)	C7—N1—Cd1—Br1	−11.1 (4)
Cd1—N3—C9—C14	−175.3 (2)	C6—N1—Cd1—Br1	158.3 (2)
C14—C9—C10—C11	1.3 (5)	C7—N1—Cd1—Br2	−133.3 (3)
N3—C9—C10—C11	−179.1 (3)	C6—N1—Cd1—Br2	36.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Br1^{i}	0.86	2.88	3.495 (4)	130

N4—H4···Br2^{ii}	0.86	2.77	3.563 (4)	155

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