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Bis[2-(1*H*-benzotriazol-1-yl)-1*H*-benzimidazol-1-ido]diethanolcadmium

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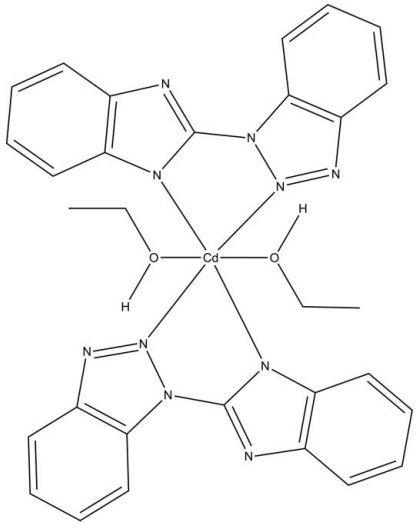
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.089; wR factor = 0.221; data-to-parameter ratio = 18.2.

In the title complex, $[Cd(C_{13}H_8N_5)_2(C_2H_5OH)_2]$, the Cd^{II} cation is located on an inversion center and coordinated by two deprotonated 2-(1*H*-benzotriazol-1-yl)-1*H*-benzimidazol-1-ide (*L*) ligands and two ethanol molecules in a distorted N_4O_2 octahedral geometry. In the *L* ligand, the dihedral angle between benzoimidazole and benzotriazole ring systems is 10.8 (3)°. In the crystal, the complex molecules are connected by O—H···N hydrogen bonds; intermolecular π–π stacking is also observed [centroid–centroid distances of 3.668 (5) Å between triazole and benzene rings and 3.780 (5) Å between imidazole rings].

Related literature

For applications of metal comlexes with heterocyclic ligands, see: Zhou *et al.* (2006); Batten & Robson (1998); Zaworotko (1994). For a related structure, see: Wu *et al.* (2009).



Experimental

Crystal data

$[Cd(C_{13}H_8N_5)_2(C_2H_6O)_2]$
M_r = 673.03
Monoclinic, $P2_1/c$
a = 8.7544 (4) Å
b = 8.0112 (2) Å
c = 20.9382 (9) Å
β = 101.352 (5)°
V = 1439.74 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.81 mm^{-1}
T = 293 K
0.32 × 0.28 × 0.25 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.773, T_{max} = 0.818
7375 measured reflections
3636 independent reflections
2781 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.089
$wR(F^2)$ = 0.221
S = 1.20
3636 reflections
200 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 2.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.97 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1	2.414 (7)	Cd1—N5	2.180 (6)
Cd1—N2	2.494 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N4^{i}	0.85 (1)	1.98 (5)	2.787 (9)	159 (12)

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The work was supported by the National Natural Science Foundation of China (Nos. 20871099 and J0730425) and Gansu Provincial Natural Science Foundation of China (No. 0710RJZA113).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5670).

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supporting information

Acta Cryst. (2013). E**69**, m134 [doi:10.1107/S1600536813001827]

Bis[2-(1*H*-benzotriazol-1-yl)-1*H*-benzimidazol-1-ido]diethanolcadmium

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S1. Comment

Over the past decades, we lay much stress on the complexation of metal ions by nitrogen heterocyclic compounds as their applications in the areas of optical, lectronic properties and magnetice (Zhou *et al.*, 2006; Batten & Robson, 1998; Zaworotko, 1994).

The title compound possesses the benzotriazole and the benzimidazole rings and can offer possibilities to form complicated coordination complexes (Wu *et al.* 2009). In the crystal, the asymmetric unit contains one half Cd^{2+} cation, one organic *L* ligands and one ethanol molecules. The Cd^{2+} is coordinated by four N atoms from two different *L* ligands and two O atoms from two ethanol molecules. Molecules are connected by O—H···N hydrogen bonds and π-π interactions [centroid–centroid distance = 3.668 (5) and 3.780 (5) Å] involving related triazole, imidazole and benzene rings.

S2. Experimental

To a yellow solution of *L* (35 mg, 0.15 mmol) and $Cd(NO_3)_2$ (52.3 mg, 0.3 mmol) in ethanol (15 ml) were placed in a Teflon lined stainless steel autoclave and heated at 120 °C for 3 days under autogenous pressure. Then it was allowed to cool to room temperature. Stick-shaped crystals were collected in 50% yield. The crystals were repeatedly washed with ethanol and air-dried.

S3. Refinement

Ethanol H atom was located in a difference Fourier map and positional parameters were refined, $U_{iso}(H) = 1.5U_{eq}(O)$. The C-bound H atoms were included in calculated position and refined in riding-model approximation with C—H = 0.93 Å, $U_{iso}(H) = 1.2U_{eq}(C)$.

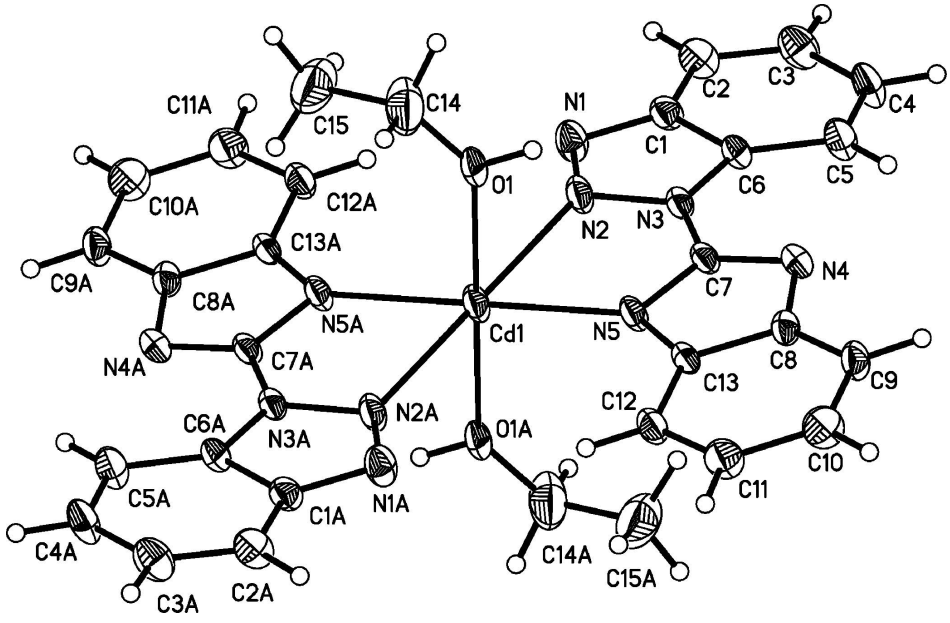

Figure 1

The molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

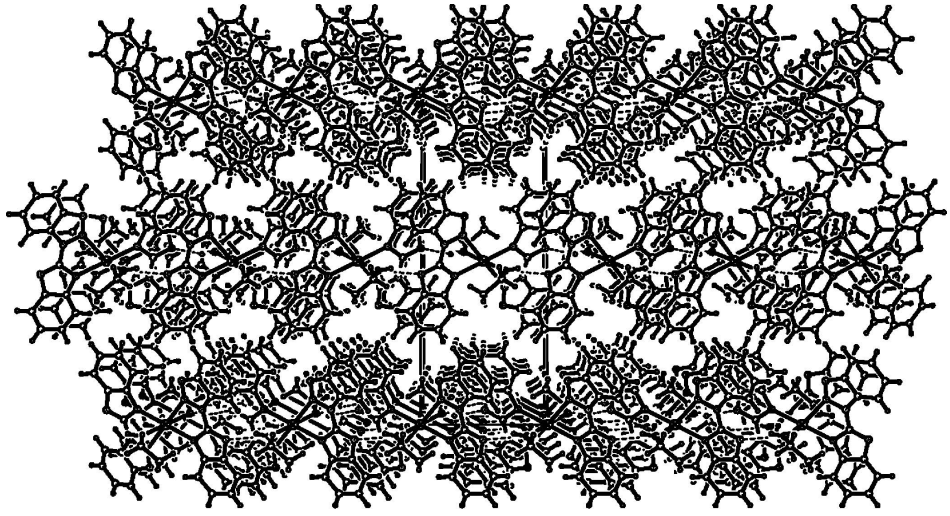

Figure 2

The crystal packing of the title compound, viewed along the *a* axis.

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Crystal data

$[Cd(C_{13}H_8N_5)_2(C_2H_6O)_2]$
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Hall symbol: -P 2ybc
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b = 8.0112 (2) Å
c = 20.9382 (9) Å
β = 101.352 (5)°
V = 1439.74 (10) Å^3
Z = 2
$F(000)$ = 684
D_x = 1.552 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3469 reflections

θ = 3.4–28.4°
μ = 0.81 mm^{-1}
T = 293 K

Block, yellow
0.32 × 0.28 × 0.25 mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0733 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.773, T_{max} = 0.818

7375 measured reflections
3636 independent reflections
2781 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 28.5°, θ_{min} = 3.4°
h = −11→11
k = −9→10
l = −26→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.089
$wR(F^2)$ = 0.221
S = 1.20
3636 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 19.0636P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 2.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.97 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.5000	0.5000	0.0382 (3)
N5	0.0518 (8)	0.2674 (8)	0.4545 (3)	0.0345 (15)
N4	0.1590 (8)	0.0074 (9)	0.4596 (3)	0.0371 (15)
C7	0.1439 (9)	0.1508 (9)	0.4883 (4)	0.0303 (15)
N2	0.1878 (9)	0.3336 (8)	0.5803 (3)	0.0397 (16)
C4	0.5416 (12)	−0.0727 (12)	0.6419 (5)	0.049 (2)
H4	0.6007	−0.1689	0.6413	0.059*
C6	0.3410 (9)	0.1084 (10)	0.5935 (4)	0.0341 (17)
C5	0.4252 (11)	−0.0382 (11)	0.5883 (5)	0.047 (2)
H5	0.4046	−0.1068	0.5518	0.057*
C3	0.5740 (11)	0.0307 (12)	0.6967 (5)	0.050 (2)
H3	0.6556	0.0032	0.7307	0.060*

C13	−0.0046 (9)	0.1884 (9)	0.3956 (4)	0.0320 (16)
O1	−0.2074 (8)	0.3361 (7)	0.5291 (4)	0.0470 (16)
H1	−0.199 (14)	0.233 (3)	0.522 (6)	0.071*
N3	0.2245 (8)	0.1886 (8)	0.5512 (3)	0.0317 (14)
C9	0.0275 (11)	−0.0769 (11)	0.3455 (4)	0.0404 (19)
H9	0.0686	−0.1842	0.3475	0.048*
C14	−0.3409 (15)	0.3597 (16)	0.5541 (8)	0.081 (4)
H14A	−0.3628	0.2586	0.5762	0.098*
H14B	−0.4281	0.3800	0.5185	0.098*
C2	0.4898 (11)	0.1690 (12)	0.7015 (5)	0.046 (2)
H2	0.5096	0.2352	0.7387	0.055*
C12	−0.1048 (11)	0.2473 (11)	0.3394 (4)	0.042 (2)
H12	−0.1483	0.3536	0.3372	0.050*
C10	−0.0704 (12)	−0.0196 (14)	0.2903 (5)	0.052 (2)
H10	−0.0937	−0.0885	0.2539	0.063*
C11	−0.1348 (12)	0.1384 (12)	0.2877 (5)	0.049 (2)
H11	−0.2010	0.1723	0.2496	0.059*
C8	0.0624 (9)	0.0309 (9)	0.3979 (4)	0.0326 (17)
C1	0.3704 (10)	0.2104 (10)	0.6481 (4)	0.0361 (17)
N1	0.2753 (9)	0.3473 (9)	0.6380 (4)	0.0430 (17)
C15	−0.3265 (19)	0.5020 (19)	0.6007 (8)	0.096 (5)
H15A	−0.3235	0.6049	0.5774	0.144*
H15B	−0.2324	0.4903	0.6328	0.144*
H15C	−0.4145	0.5027	0.6218	0.144*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0529 (5)	0.0192 (4)	0.0413 (5)	0.0066 (4)	0.0064 (4)	−0.0031 (4)
N5	0.046 (4)	0.017 (3)	0.039 (4)	0.004 (3)	0.004 (3)	0.001 (3)
N4	0.045 (4)	0.026 (3)	0.041 (4)	0.006 (3)	0.008 (3)	0.007 (3)
C7	0.035 (4)	0.018 (3)	0.038 (4)	0.000 (3)	0.008 (3)	0.004 (3)
N2	0.057 (4)	0.022 (3)	0.039 (4)	0.010 (3)	0.006 (3)	−0.003 (3)
C4	0.058 (6)	0.030 (4)	0.053 (6)	0.013 (4)	−0.005 (4)	0.003 (4)
C6	0.041 (4)	0.020 (3)	0.041 (4)	0.000 (3)	0.010 (3)	0.002 (3)
C5	0.055 (5)	0.032 (5)	0.053 (5)	0.009 (4)	0.005 (4)	0.001 (4)
C3	0.049 (5)	0.043 (6)	0.052 (5)	0.001 (4)	−0.006 (4)	0.004 (4)
C13	0.043 (4)	0.020 (3)	0.033 (4)	0.005 (3)	0.007 (3)	0.004 (3)
O1	0.064 (4)	0.019 (3)	0.064 (4)	0.007 (3)	0.027 (3)	−0.001 (3)
N3	0.044 (4)	0.019 (3)	0.032 (3)	0.003 (3)	0.008 (3)	0.000 (3)
C9	0.057 (5)	0.027 (4)	0.035 (4)	0.009 (4)	0.004 (4)	−0.007 (3)
C14	0.070 (8)	0.053 (7)	0.130 (12)	0.010 (6)	0.042 (8)	−0.007 (8)
C2	0.054 (5)	0.039 (5)	0.040 (5)	−0.004 (4)	−0.003 (4)	−0.002 (4)
C12	0.059 (5)	0.029 (4)	0.035 (4)	0.013 (4)	0.005 (4)	0.004 (3)
C10	0.066 (6)	0.049 (6)	0.038 (5)	−0.003 (5)	0.001 (4)	−0.008 (5)
C11	0.061 (6)	0.045 (5)	0.036 (5)	0.003 (5)	−0.001 (4)	−0.001 (4)
C8	0.037 (4)	0.024 (4)	0.037 (4)	0.001 (3)	0.008 (3)	−0.005 (3)
C1	0.046 (4)	0.028 (4)	0.033 (4)	−0.001 (3)	0.005 (3)	0.000 (3)

N1	0.056 (4)	0.032 (4)	0.035 (4)	0.007 (3)	−0.004 (3)	−0.007 (3)
C15	0.122 (12)	0.065 (8)	0.120 (12)	−0.018 (9)	0.074 (10)	−0.029 (9)

Geometric parameters (Å, º)

Cd1—O1^{i}	2.414 (7)	C13—C8	1.388 (10)
Cd1—O1	2.414 (7)	C13—C12	1.404 (11)
Cd1—N2	2.494 (7)	O1—C14	1.384 (13)
Cd1—N2^{i}	2.494 (7)	O1—H1	0.848 (10)
Cd1—N5^{i}	2.180 (6)	C9—C10	1.375 (13)
Cd1—N5	2.180 (6)	C9—C8	1.382 (11)
N5—C7	1.341 (10)	C9—H9	0.9300
N5—C13	1.388 (10)	C14—C15	1.489 (18)
N4—C7	1.316 (10)	C14—H14A	0.9700
N4—C8	1.411 (10)	C14—H14B	0.9700
C7—N3	1.399 (10)	C2—C1	1.411 (12)
N2—N1	1.301 (10)	C2—H2	0.9300
N2—N3	1.380 (9)	C12—C11	1.374 (13)
C4—C5	1.387 (13)	C12—H12	0.9300
C4—C3	1.398 (14)	C10—C11	1.383 (14)
C4—H4	0.9300	C10—H10	0.9300
C6—N3	1.371 (10)	C11—H11	0.9300
C6—C1	1.388 (11)	C1—N1	1.368 (11)
C6—C5	1.402 (11)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C3—C2	1.346 (13)	C15—H15C	0.9600
C3—H3	0.9300		

N5^{i}—Cd1—N5	180.000 (1)	C8—C13—N5	108.1 (7)
N5^{i}—Cd1—O1^{i}	82.9 (2)	C8—C13—C12	121.6 (8)
N5—Cd1—O1^{i}	97.1 (2)	N5—C13—C12	130.2 (7)
N5^{i}—Cd1—O1	97.1 (2)	C14—O1—Cd1	138.9 (7)
N5—Cd1—O1	82.9 (2)	C14—O1—H1	108 (8)
O1^{i}—Cd1—O1	180.0 (2)	Cd1—O1—H1	113 (8)
N5^{i}—Cd1—N2	109.2 (2)	C6—N3—N2	108.5 (6)
N5—Cd1—N2	70.8 (2)	C6—N3—C7	132.8 (7)
O1^{i}—Cd1—N2	91.8 (2)	N2—N3—C7	118.7 (6)
O1—Cd1—N2	88.2 (2)	C10—C9—C8	117.5 (8)
N5^{i}—Cd1—N2^{i}	70.8 (2)	C10—C9—H9	121.2
N5—Cd1—N2^{i}	109.2 (2)	C8—C9—H9	121.2
O1^{i}—Cd1—N2^{i}	88.2 (2)	O1—C14—C15	112.6 (11)
O1—Cd1—N2^{i}	91.8 (2)	O1—C14—H14A	109.1
N2—Cd1—N2^{i}	180.0 (3)	C15—C14—H14A	109.1
C7—N5—C13	102.9 (6)	O1—C14—H14B	109.1
C7—N5—Cd1	121.3 (5)	C15—C14—H14B	109.1
C13—N5—Cd1	135.2 (5)	H14A—C14—H14B	107.8
C7—N4—C8	101.9 (6)	C3—C2—C1	117.8 (9)
N4—C7—N5	118.1 (7)	C3—C2—H2	121.1

N4—C7—N3	122.8 (7)	C1—C2—H2	121.1
N5—C7—N3	119.1 (7)	C11—C12—C13	115.9 (8)
N1—N2—N3	109.6 (6)	C11—C12—H12	122.0
N1—N2—Cd1	140.4 (5)	C13—C12—H12	122.0
N3—N2—Cd1	109.4 (5)	C9—C10—C11	121.4 (9)
C5—C4—C3	123.0 (9)	C9—C10—H10	119.3
C5—C4—H4	118.5	C11—C10—H10	119.3
C3—C4—H4	118.5	C12—C11—C10	122.5 (9)
N3—C6—C1	104.5 (7)	C12—C11—H11	118.7
N3—C6—C5	132.7 (8)	C10—C11—H11	118.7
C1—C6—C5	122.8 (8)	C9—C8—C13	121.0 (8)
C4—C5—C6	114.7 (9)	C9—C8—N4	130.0 (7)
C4—C5—H5	122.7	C13—C8—N4	109.0 (7)
C6—C5—H5	122.7	N1—C1—C6	109.6 (7)
C2—C3—C4	121.5 (9)	N1—C1—C2	130.1 (8)
C2—C3—H3	119.2	C6—C1—C2	120.2 (8)
C4—C3—H3	119.2	N2—N1—C1	107.8 (7)

N5^{i}—Cd1—N5—C7	32 (100)	N2^{i}—Cd1—O1—C14	−59.3 (13)
O1^{i}—Cd1—N5—C7	93.0 (6)	C1—C6—N3—N2	0.3 (9)
O1—Cd1—N5—C7	−87.0 (6)	C5—C6—N3—N2	−177.3 (9)
N2—Cd1—N5—C7	3.5 (6)	C1—C6—N3—C7	180.0 (8)
N2^{i}—Cd1—N5—C7	−176.5 (6)	C5—C6—N3—C7	2.4 (15)
N5^{i}—Cd1—N5—C13	−158 (100)	N1—N2—N3—C6	0.1 (9)
O1^{i}—Cd1—N5—C13	−97.4 (8)	Cd1—N2—N3—C6	173.1 (5)
O1—Cd1—N5—C13	82.6 (8)	N1—N2—N3—C7	−179.6 (7)
N2—Cd1—N5—C13	173.2 (8)	Cd1—N2—N3—C7	−6.6 (8)
N2^{i}—Cd1—N5—C13	−6.8 (8)	N4—C7—N3—C6	7.9 (13)
C8—N4—C7—N5	−0.4 (9)	N5—C7—N3—C6	−169.3 (8)
C8—N4—C7—N3	−177.7 (7)	N4—C7—N3—N2	−172.5 (7)
C13—N5—C7—N4	1.5 (10)	N5—C7—N3—N2	10.3 (11)
Cd1—N5—C7—N4	174.0 (5)	Cd1—O1—C14—C15	−33 (2)
C13—N5—C7—N3	178.8 (7)	C4—C3—C2—C1	−2.2 (15)
Cd1—N5—C7—N3	−8.6 (10)	C8—C13—C12—C11	1.5 (13)
N5^{i}—Cd1—N2—N1	−8.7 (10)	N5—C13—C12—C11	178.0 (9)
N5—Cd1—N2—N1	171.3 (10)	C8—C9—C10—C11	−1.7 (15)
O1^{i}—Cd1—N2—N1	74.5 (10)	C13—C12—C11—C10	−0.3 (15)
O1—Cd1—N2—N1	−105.5 (10)	C9—C10—C11—C12	0.4 (17)
N2^{i}—Cd1—N2—N1	130 (100)	C10—C9—C8—C13	2.8 (13)
N5^{i}—Cd1—N2—N3	−178.2 (5)	C10—C9—C8—N4	−179.3 (9)
N5—Cd1—N2—N3	1.8 (5)	N5—C13—C8—C9	180.0 (8)
O1^{i}—Cd1—N2—N3	−95.1 (5)	C12—C13—C8—C9	−2.8 (13)
O1—Cd1—N2—N3	84.9 (5)	N5—C13—C8—N4	1.7 (9)
N2^{i}—Cd1—N2—N3	−39 (100)	C12—C13—C8—N4	178.9 (8)
C3—C4—C5—C6	−0.5 (15)	C7—N4—C8—C9	−178.9 (9)
N3—C6—C5—C4	176.7 (9)	C7—N4—C8—C13	−0.8 (9)
C1—C6—C5—C4	−0.6 (13)	N3—C6—C1—N1	−0.7 (9)
C5—C4—C3—C2	2.1 (17)	C5—C6—C1—N1	177.3 (8)

C7—N5—C13—C8	−1.9 (9)	N3—C6—C1—C2	−177.6 (8)
Cd1—N5—C13—C8	−172.8 (6)	C5—C6—C1—C2	0.4 (13)
C7—N5—C13—C12	−178.7 (9)	C3—C2—C1—N1	−175.1 (9)
Cd1—N5—C13—C12	10.3 (14)	C3—C2—C1—C6	1.1 (14)
N5^{i}—Cd1—O1—C14	11.6 (13)	N3—N2—N1—C1	−0.5 (10)
N5—Cd1—O1—C14	−168.4 (13)	Cd1—N2—N1—C1	−170.1 (7)
O1^{i}—Cd1—O1—C14	−110 (100)	C6—C1—N1—N2	0.7 (10)
N2—Cd1—O1—C14	120.7 (13)	C2—C1—N1—N2	177.2 (9)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N4^{ii}	0.85 (1)	1.98 (5)	2.787 (9)	159 (12)

Symmetry code: (ii) −*x*, −*y*, −*z*+1.