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catena-Poly[[aqua(imidazole)-cadmium(II)]-μ_3-benzene-1,3-dicarboxylato]

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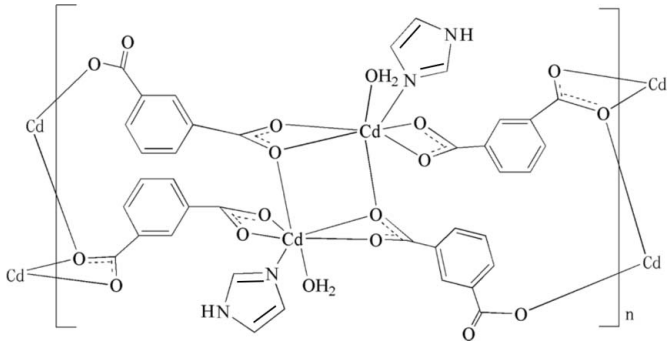
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.028; wR factor = 0.072; data-to-parameter ratio = 11.3.

In the title compound, $[Cd(C_8H_4O_4)(C_3H_4N_2)(H_2O)]_n$, the Cd^{II} ion is seven-coordinated by five O atoms from three crystallographically independent benzene-1,3-carboxylate ligands, one N atom from the imidazole ligand and one coordinated water molecule. Neighboring Cd^{II} ions are bridged by the benzene-1,3-dicarboxylate ligands, forming a zigzag polymeric chain structure. These chains are further extended into a three-dimensional supramolecular structure through O—H···O and N—H···O hydrogen bonds.

Related literature

For the synthesis, see: Yaghi *et al.* (1998). For related structures, see: Ma *et al.* (2008); Wang *et al.* (2008).



Experimental

Crystal data

$[Cd(C_8H_4O_4)(C_3H_4N_2)(H_2O)]$
M_r = 362.61
Triclinic, $P\overline{1}$
a = 8.2616 (8) Å
b = 8.3138 (8) Å
c = 10.235 (1) Å
α = 67.017 (2)°
β = 68.176 (2)°
γ = 81.054 (2)°
V = 600.76 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.84 mm^{-1}
T = 293 K
0.27 × 0.18 × 0.06 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.536, T_{max} = 1.000
3166 measured reflections
2086 independent reflections
2049 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.15
2086 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.216 (3)	Cd1—O1	2.413 (3)
Cd1—O3^{i}	2.251 (3)	Cd1—O1^{ii}	2.626 (3)
Cd1—O2^{ii}	2.311 (3)	Cd1—O4^{i}	2.663 (3)
Cd1—O5	2.394 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O2^{iii}	0.84 (8)	2.07 (8)	2.809 (4)	146 (7)
O5—H5B···O3^{iv}	0.87 (8)	1.96 (8)	2.786 (4)	158 (7)
N2—H2···O4^{v}	0.85 (7)	2.00 (7)	2.854 (5)	175 (6)

Symmetry codes: (iii) $x, y-1, z$; (iv) $x, y-1, z+1$; (v) $x+1, y, z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: LX2148).

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catena-Poly[[aqua(imidazole)cadmium(II)]-μ_3-benzene-1,3-dicarboxylato]

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S1. Comment

In recent years, considerable effort was paied in the study of metal-organic hybrid materials with the extended supermolecular framework structures, owing to their intriguing network topologies and potential application in adsorption, molecular recognition, catalysis and maganetism (Yaghi *et al.*, 1998). Currently, carboxylic acids have been widely used as polydentate and bridging ligands since they can bind metal ions in diverse modes and play an important role in adjusting verious topologies structures. A number of promising supramolecular complexes have been designed and constructed by using carboxylic acids as favorable conditions. (Ma *et al.*, 2008; Wang *et al.*, 2008). In this paper, we report the synthesis and structural characterzation of the title compound in which the isophthalic acid ligand displayed its good coordination ability and diverse coordination modes.

The Cd^{II} ion is six-coordinated by four O atoms from three crystallographically independent benzene-1,3- dicarboxylate ligands and one N atom from the chelating imidazole ligand and one coordinated water molecule (Fig. 1 & Table 1). The neighboring Cd^{i} ion is bridged by the benzene-1, 3-dicarboxylate ligands to form a one-dimensional chain structure. In the crystal structure, the adjacent chains are linked *via* O–H···O and N–H···O hydrogen bonds (Fig. 2 & Table 2) resulting in the formation of a three dimensional supramolecular structure.

S2. Experimental

A 10 ml aqueous solution of imidazole (0.014 g, 0.20 mmol) and isophthalic acid (0.034 g,0.020 *m*mol) was slowly added into cadmium nitrate (0.062 g, 0.20 *m*mol) solution in methanol (10 ml), and the mixed solution was stirred for 20 min and then was heated in a 30 ml Teflon-line autoclave under autogeneous pressure at 423 K for 3 d. After cooling to room temperature, colorless block crystals were obtained. (yield 38%).

S3. Refinement

H atoms bound to H_2O and NH atoms were located in a difference map and refined freely. Other H atoms were positioned geometrically and refined using a riding model, with C–H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

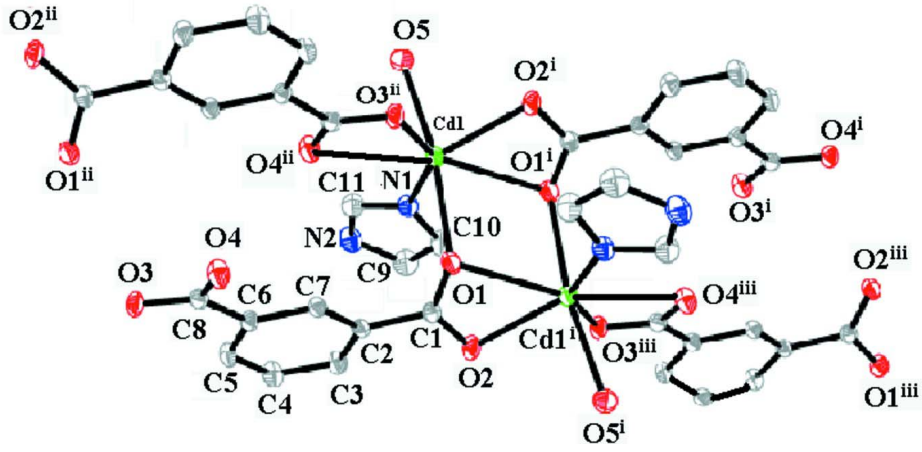

Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. [Symmetry codes: (i) -*x*, -*y*+1, -*z*+2; (ii) -*x*, -*y*+1, -*z*+1; (iii) *x*, *y*, *z*+1.]

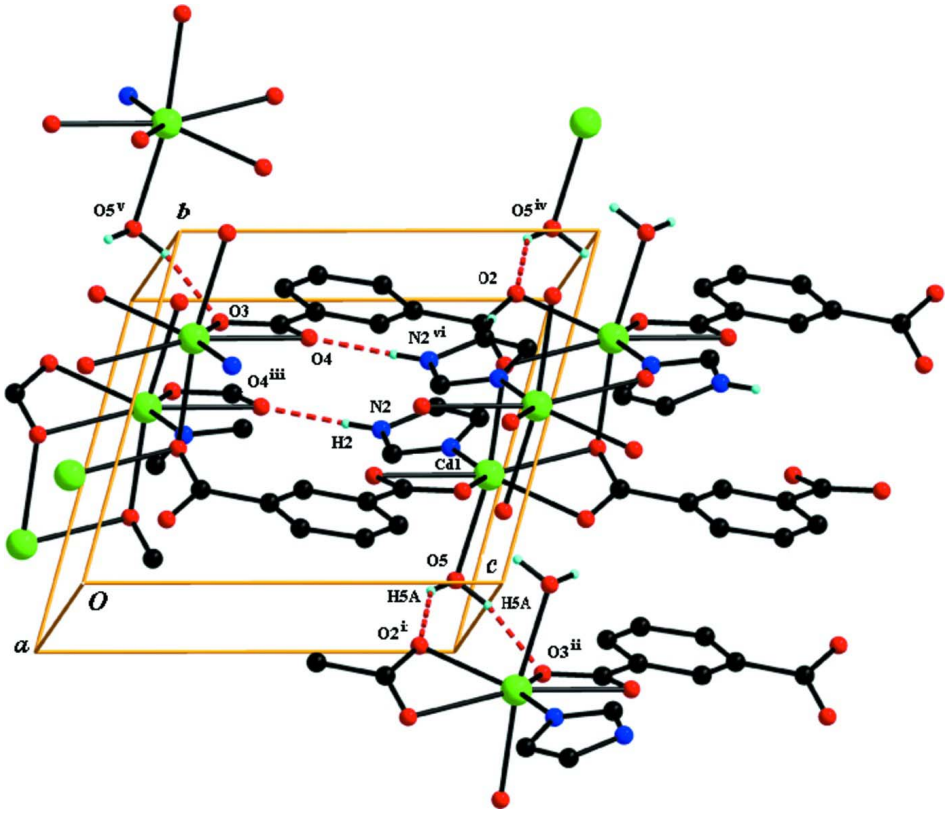

Figure 2

The crystal packing of (I), showing one layer of molecules connected by O–H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (i) *x*, *y*-1 , *z*; (ii) *x*, *y*-1, *z*+1; (iii) *x*+1, *y*, *z*; (iv) -*x*, -*y*+1, -*z*+1; (v) -*x*, -*y*+1, -*z*+2.]

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Crystal data

$[Cd(C_8H_4O_4)(C_3H_4N_2)(H_2O)]$
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Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.2616 (8) Å
b = 8.3138 (8) Å
c = 10.235 (1) Å
α = 67.017 (2)°
β = 68.176 (2)°
γ = 81.054 (2)°
V = 600.76 (10) Å^3
Z = 2
F(000) = 356
D_x = 2.005 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3126 reflections
θ = 3.3–27.5°
μ = 1.84 mm^{-1}
T = 293 K
Block, yellow
0.27 × 0.18 × 0.06 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.536, T_{max} = 1.000
3166 measured reflections
2086 independent reflections
2049 reflections with $I > 2\sigma(I)$

R_{int} = 0.019
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −9→9
k = −9→4
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.072
S = 1.15
2086 reflections
184 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 1.1125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	0.08672 (3)	0.32297 (3)	0.90289 (3)	0.02898 (11)
O1	−0.0532 (4)	0.6070 (4)	0.8593 (3)	0.0337 (6)
O2	0.0672 (4)	0.8334 (4)	0.8475 (3)	0.0382 (6)
O3	0.1082 (4)	0.7617 (4)	0.1628 (3)	0.0347 (6)
O4	−0.1232 (4)	0.6718 (4)	0.3685 (3)	0.0405 (7)
O5	0.2389 (4)	0.0533 (4)	0.9029 (4)	0.0414 (7)
H5A	0.209 (10)	0.017 (10)	0.849 (9)	0.10 (2)*
H5B	0.211 (10)	−0.024 (10)	0.994 (9)	0.10 (3)*
N1	0.3422 (4)	0.4507 (4)	0.8114 (4)	0.0340 (7)
N2	0.5999 (5)	0.5524 (5)	0.6516 (4)	0.0453 (9)
H2	0.687 (9)	0.587 (9)	0.570 (8)	0.08 (2)*
C1	0.0393 (5)	0.7429 (5)	0.7840 (4)	0.0272 (7)
C2	0.1174 (5)	0.7962 (5)	0.6165 (4)	0.0255 (7)
C3	0.2660 (5)	0.8979 (5)	0.5366 (4)	0.0325 (8)
H3	0.3153	0.9372	0.5868	0.039*
C4	0.3406 (5)	0.9406 (6)	0.3814 (5)	0.0398 (9)
H4	0.4428	1.0048	0.3284	0.048*
C5	0.2642 (5)	0.8885 (5)	0.3047 (4)	0.0333 (8)
H5	0.3145	0.9184	0.2006	0.040*
C8	0.0251 (5)	0.7384 (5)	0.3016 (4)	0.0293 (8)
C7	0.0420 (4)	0.7439 (4)	0.5394 (4)	0.0248 (7)
H7	−0.0575	0.6757	0.5930	0.030*

C11	0.4652 (6)	0.4570 (6)	0.6844 (5)	0.0425 (10)
H11	0.4592	0.4010	0.6235	0.051*
C10	0.4032 (6)	0.5481 (6)	0.8641 (5)	0.0436 (10)
H10	0.3441	0.5688	0.9532	0.052*
C9	0.5632 (6)	0.6097 (7)	0.7663 (6)	0.0488 (11)
H9	0.6338	0.6779	0.7762	0.059*
C6	0.1121 (5)	0.7914 (5)	0.3837 (4)	0.0261 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03179 (17)	0.03293 (17)	0.02429 (16)	−0.01047 (11)	−0.00754 (11)	−0.01069 (12)
O1	0.0381 (15)	0.0359 (15)	0.0243 (13)	−0.0070 (12)	−0.0089 (11)	−0.0074 (11)
O2	0.0528 (17)	0.0447 (16)	0.0260 (13)	−0.0095 (13)	−0.0144 (12)	−0.0175 (12)
O3	0.0442 (15)	0.0420 (15)	0.0236 (13)	−0.0069 (12)	−0.0114 (11)	−0.0154 (11)
O4	0.0422 (16)	0.0530 (18)	0.0302 (14)	−0.0195 (13)	−0.0118 (12)	−0.0125 (13)
O5	0.0440 (17)	0.0385 (16)	0.0405 (17)	−0.0083 (13)	−0.0105 (14)	−0.0137 (15)
N1	0.0310 (16)	0.0374 (18)	0.0328 (17)	−0.0080 (13)	−0.0085 (13)	−0.0114 (14)
N2	0.0336 (19)	0.055 (2)	0.039 (2)	−0.0110 (17)	−0.0046 (16)	−0.0120 (18)
C1	0.0274 (18)	0.0310 (19)	0.0236 (17)	−0.0004 (14)	−0.0103 (14)	−0.0091 (15)
C2	0.0289 (18)	0.0254 (17)	0.0223 (17)	−0.0011 (14)	−0.0100 (14)	−0.0073 (14)
C3	0.036 (2)	0.042 (2)	0.0276 (19)	−0.0122 (16)	−0.0133 (16)	−0.0137 (16)
C4	0.033 (2)	0.053 (3)	0.032 (2)	−0.0214 (18)	−0.0048 (16)	−0.0118 (18)
C5	0.035 (2)	0.042 (2)	0.0202 (17)	−0.0076 (16)	−0.0060 (15)	−0.0092 (16)
C8	0.038 (2)	0.0273 (18)	0.0267 (18)	−0.0028 (15)	−0.0152 (16)	−0.0089 (15)
C7	0.0250 (17)	0.0278 (17)	0.0220 (17)	−0.0045 (13)	−0.0084 (13)	−0.0075 (14)
C11	0.040 (2)	0.050 (3)	0.040 (2)	−0.0124 (19)	−0.0100 (18)	−0.017 (2)
C10	0.036 (2)	0.057 (3)	0.042 (2)	−0.0128 (19)	−0.0100 (18)	−0.021 (2)
C9	0.040 (2)	0.057 (3)	0.054 (3)	−0.017 (2)	−0.015 (2)	−0.020 (2)
C6	0.0285 (18)	0.0281 (18)	0.0248 (17)	−0.0013 (14)	−0.0113 (14)	−0.0105 (14)

Geometric parameters (Å, º)

Cd1—N1	2.216 (3)	N2—H2	0.85 (7)
Cd1—O3^{i}	2.251 (3)	C1—C2	1.492 (5)
Cd1—O2^{ii}	2.311 (3)	C2—C7	1.384 (5)
Cd1—O5	2.394 (3)	C2—C3	1.388 (5)
Cd1—O1	2.413 (3)	C3—C4	1.389 (5)
Cd1—O1^{ii}	2.626 (3)	C3—H3	0.9300
Cd1—O4^{i}	2.663 (3)	C4—C5	1.387 (6)
O1—C1	1.266 (5)	C4—H4	0.9300
O2—C1	1.260 (4)	C5—C6	1.391 (5)
O3—C8	1.276 (4)	C5—H5	0.9300
O4—C8	1.252 (5)	C8—C6	1.501 (5)
O5—H5A	0.84 (8)	C7—C6	1.387 (5)
O5—H5B	0.87 (8)	C7—H7	0.9300
N1—C11	1.306 (5)	C11—H11	0.9300
N1—C10	1.368 (5)	C10—C9	1.356 (6)

N2—C11	1.330 (6)	C10—H10	0.9300
N2—C9	1.351 (6)	C9—H9	0.9300

N1—Cd1—O3^{i}	143.34 (11)	C9—N2—H2	124 (4)
N1—Cd1—O2^{ii}	127.43 (11)	O2—C1—O1	121.5 (3)
O3^{i}—Cd1—O2^{ii}	88.49 (10)	O2—C1—C2	119.4 (3)
N1—Cd1—O5	88.63 (11)	O1—C1—C2	119.1 (3)
O3^{i}—Cd1—O5	87.33 (11)	C7—C2—C3	119.4 (3)
O2^{ii}—Cd1—O5	85.20 (11)	C7—C2—C1	120.0 (3)
N1—Cd1—O1	89.20 (11)	C3—C2—C1	120.5 (3)
O3^{i}—Cd1—O1	89.03 (10)	C2—C3—C4	119.7 (3)
O2^{ii}—Cd1—O1	103.25 (10)	C2—C3—H3	120.2
O5—Cd1—O1	170.71 (11)	C4—C3—H3	120.2
N1—Cd1—O1^{ii}	83.08 (10)	C5—C4—C3	120.6 (4)
O3^{i}—Cd1—O1^{ii}	131.61 (9)	C5—C4—H4	119.7
O2^{ii}—Cd1—O1^{ii}	52.58 (9)	C3—C4—H4	119.7
O5—Cd1—O1^{ii}	112.79 (11)	C4—C5—C6	119.8 (3)
O1—Cd1—O1^{ii}	75.89 (9)	C4—C5—H5	120.1
N1—Cd1—O4^{i}	91.00 (10)	C6—C5—H5	120.1
O3^{i}—Cd1—O4^{i}	52.54 (9)	O4—C8—O3	121.5 (3)
O2^{ii}—Cd1—O4^{i}	137.72 (9)	O4—C8—C6	120.7 (3)
O5—Cd1—O4^{i}	78.09 (11)	O3—C8—C6	117.8 (3)
O1—Cd1—O4^{i}	92.92 (9)	C2—C7—C6	121.2 (3)
O1^{ii}—Cd1—O4^{i}	167.35 (9)	C2—C7—H7	119.4
C1—O1—Cd1	119.5 (2)	C6—C7—H7	119.4
C1—O1—Cd1^{ii}	85.5 (2)	N1—C11—N2	112.7 (4)
Cd1—O1—Cd1^{ii}	104.11 (9)	N1—C11—H11	123.7
C1—O2—Cd1^{ii}	100.4 (2)	N2—C11—H11	123.7
C8—O3—Cd1^{i}	102.2 (2)	C9—C10—N1	109.4 (4)
Cd1—O5—H5A	108 (5)	C9—C10—H10	125.3
Cd1—O5—H5B	110 (5)	N1—C10—H10	125.3
H5A—O5—H5B	109 (7)	N2—C9—C10	106.5 (4)
C11—N1—C10	104.7 (3)	N2—C9—H9	126.7
C11—N1—Cd1	125.3 (3)	C10—C9—H9	126.7
C10—N1—Cd1	129.8 (3)	C7—C6—C5	119.1 (3)
C11—N2—C9	106.7 (4)	C7—C6—C8	120.4 (3)
C11—N2—H2	129 (4)	C5—C6—C8	120.4 (3)

N1—Cd1—O1—C1	9.8 (3)	O2—C1—C2—C7	−156.1 (3)
O3^{i}—Cd1—O1—C1	−133.6 (3)	O1—C1—C2—C7	24.1 (5)
O2^{ii}—Cd1—O1—C1	138.2 (3)	O2—C1—C2—C3	24.1 (5)
O1^{ii}—Cd1—O1—C1	92.8 (3)	O1—C1—C2—C3	−155.6 (4)
O4^{i}—Cd1—O1—C1	−81.2 (3)	C7—C2—C3—C4	−2.3 (6)
N1—Cd1—O1—Cd1^{ii}	−83.06 (11)	C1—C2—C3—C4	177.5 (4)
O3^{i}—Cd1—O1—Cd1^{ii}	133.56 (10)	C2—C3—C4—C5	2.6 (7)
O2^{ii}—Cd1—O1—Cd1^{ii}	45.34 (11)	C3—C4—C5—C6	−0.5 (7)
O1^{ii}—Cd1—O1—Cd1^{ii}	0.0	Cd1^{i}—O3—C8—O4	4.2 (4)
O4^{i}—Cd1—O1—Cd1^{ii}	−174.03 (9)	Cd1^{i}—O3—C8—C6	−176.6 (3)

O3^{i}—Cd1—N1—C11	−24.3 (5)	C3—C2—C7—C6	−0.1 (5)
O2^{ii}—Cd1—N1—C11	142.2 (3)	C1—C2—C7—C6	−179.9 (3)
O5—Cd1—N1—C11	59.3 (4)	C10—N1—C11—N2	−0.4 (5)
O1—Cd1—N1—C11	−111.6 (4)	Cd1—N1—C11—N2	175.6 (3)
O1^{ii}—Cd1—N1—C11	172.5 (4)	C9—N2—C11—N1	1.0 (6)
O4^{i}—Cd1—N1—C11	−18.7 (4)	C11—N1—C10—C9	−0.4 (5)
O3^{i}—Cd1—N1—C10	150.6 (3)	Cd1—N1—C10—C9	−176.1 (3)
O2^{ii}—Cd1—N1—C10	−42.9 (4)	C11—N2—C9—C10	−1.2 (5)
O5—Cd1—N1—C10	−125.8 (4)	N1—C10—C9—N2	0.9 (6)
O1—Cd1—N1—C10	63.3 (4)	C2—C7—C6—C5	2.1 (5)
O1^{ii}—Cd1—N1—C10	−12.6 (4)	C2—C7—C6—C8	−178.0 (3)
O4^{i}—Cd1—N1—C10	156.2 (4)	C4—C5—C6—C7	−1.8 (6)
Cd1^{ii}—O2—C1—O1	0.1 (4)	C4—C5—C6—C8	178.3 (4)
Cd1^{ii}—O2—C1—C2	−179.6 (3)	O4—C8—C6—C7	9.7 (5)
Cd1—O1—C1—O2	−103.8 (4)	O3—C8—C6—C7	−169.4 (3)
Cd1^{ii}—O1—C1—O2	−0.1 (3)	O4—C8—C6—C5	−170.4 (4)
Cd1—O1—C1—C2	76.0 (4)	O3—C8—C6—C5	10.4 (5)
Cd1^{ii}—O1—C1—C2	179.6 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O2^{iii}	0.84 (8)	2.07 (8)	2.809 (4)	146 (7)
O5—H5*B*···O3^{iv}	0.87 (8)	1.96 (8)	2.786 (4)	158 (7)
N2—H2···O4^{v}	0.85 (7)	2.00 (7)	2.854 (5)	175 (6)

Symmetry codes: (iii) *x*, *y*−1, *z*; (iv) *x*, *y*−1, *z*+1; (v) *x*+1, *y*, *z*.