Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[aqua(1-naphthylacetato)-cadmium(II)]-μ_3-pyridin-3-olato]

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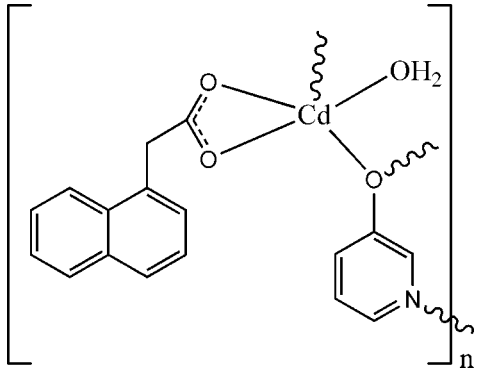
Received 8 November 2007; accepted 22 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 16.9.

In the title complex, $[Cd(C_5H_4NO)(C_{12}H_9O_2)(H_2O)]_n$, each Cd^{II} atom is coordinated by two carboxylate O atoms from one 1-naphthylacetate ligand, two hydroxyl O atoms from two pyridin-3-olate ligands, one N atom from another pyridin-3-olate ligand and one water molecule, and displays a distorted octahedral coordination geometry. The compound forms infinite chains of pyridin-3-olate ligands bridging 1-naphthylacetate–Cd^{II} units parallel to the b axis, with a Cd···Cd separation of 3.578 (2) Å. The chains are further self-assembled into a supramolecular network through intermolecular O—H···O hydrogen-bonding interactions.

Related literature

Other structures of naphthylacetic acid have been reported by Chen *et al.* (2004); Duan *et al.* (2007); Liu *et al.* (2006); and Tang *et al.* (2006).



Experimental

Crystal data

$[Cd(C_5H_4NO)(C_{12}H_9O_2)(H_2O)]$
M_r = 409.70
Monoclinic, $P2_1/c$
a = 14.978 (2) Å
b = 6.7324 (1) Å
c = 15.729 (2) Å
β = 95.928 (1)°
V = 1577.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 296 (2) K
0.26 × 0.23 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.702, T_{max} = 0.757
16642 measured reflections
3617 independent reflections
3172 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.066
S = 1.05
3617 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O1^{i}	0.75 (3)	1.97 (3)	2.720 (3)	174 (4)
O1W—H2W···O2^{ii}	0.77 (3)	2.02 (3)	2.783 (3)	173 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Dong Hua University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2087).

References

Bruker (2004). *APEX2* (Version 7.23A), *SAINT* (Version 7.23A) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, L.-F., Zhang, J., Song, L.-J., Wang, W.-G. & Ju, Z.-F. (2004). *Acta Cryst.* E**60**, m1032–m1034.
Duan, J.-G., Liu, J.-W. & Wu, S. (2007). *Acta Cryst.* E**63**, m692–m694.
Liu, J.-W., Wang, W.-Y. & Gu, C.-S. (2006). *Acta Cryst.* E**62**, m3445–m3447.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Tang, D. X., Feng, L. X. & Zhang, X. Q. (2006). *Chin. J. Inorg. Chem.* **22**, 1891–1894.

 doi:10.1107/S1600536807062332

supporting information

Acta Cryst. (2008). E**64**, m31 [https://doi.org/10.1107/S1600536807062332]

Poly[[aqua(1-naphthylacetato)cadmium(II)]-μ_3-pyridin-3-olato]

Chun-Yan Ma, Wen-Dong Song and Dan-Li Xi

S1. Comment

In structural investigations of complexes containing the 1-naphthylacetic acid ligand, it has been found that this molecule can act as a multidentate ligand with a range of versatile binding and coordination modes (Chen *et al.*, 2004; Duan *et al.*, 2007; Liu *et al.*, 2006; Tang *et al.*, 2006). In this paper, we report the crystal structure of the a new Cd complex obtained by the reaction of 1-naphthylacetic acid, 3-hydroxypyridine and cadmium chloride in alkaline aqueous solution.

As illustrated in Figure 1, each Cd^{II} atom, has a distorted octahedral geometry with the six coordinating atoms being two carboxyl O atoms from one 1-naphthylacetate ligands, two hydroxyl O atoms from two pyridin-3-olate ligands, one N atom from another pyridin-3-olate ligand and one water molecule. The pyridin-3-olate ligands connect 1-naphthylacetate-Cd^{II} units to form an infinite chain parallel to the *b* axis with a Cd···Cd separation of 3.578 (2) Å. These chains are further assembled by intermolecular O—H···O hydrogen bonding, with the coordinating water molecules as donors and the carboxyl O atoms as acceptors, thus forming a supramolecular network (Fig. 2).

S2. Experimental

A mixture of cadmium chloride (1 mmol), 3-hydroxypyridine (1 mmol), 1-naphthylacetic acid (1 mmol), NaOH (1.5 mmol) and H_2O (12 ml) was placed in a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The crystals obtained were washed with water and dryed in air.

S3. Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2 U_{eq}(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å and H···H = 1.29 Å, each within a standard deviation of 0.01 Å with U_{iso}(H) = 1.5 U_{eq}(O).

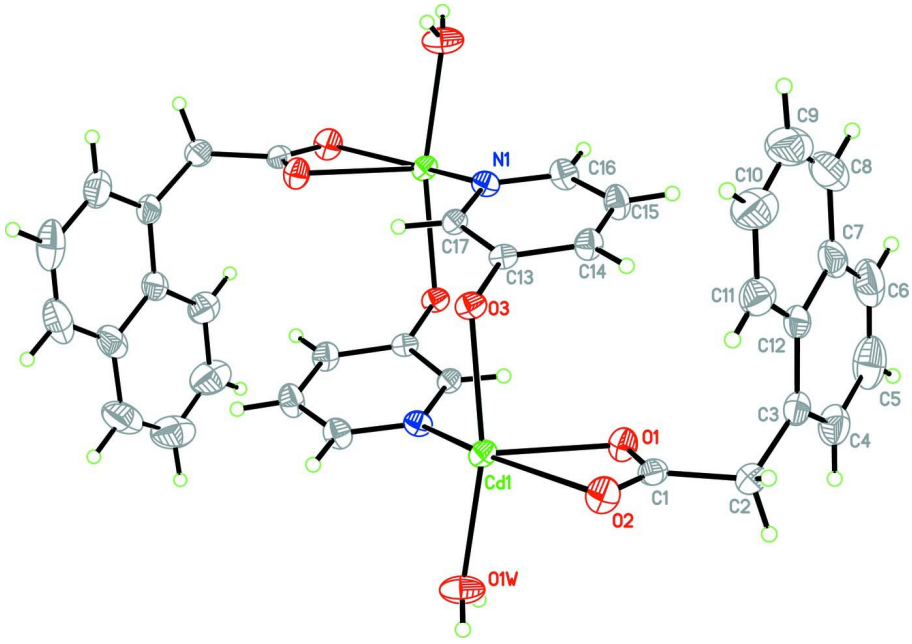


Figure 1

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids. Unlabeled atoms are related to the labelled atoms by the symmetry operator (1 - *x*, 2 - *y*, 1 - *z*).

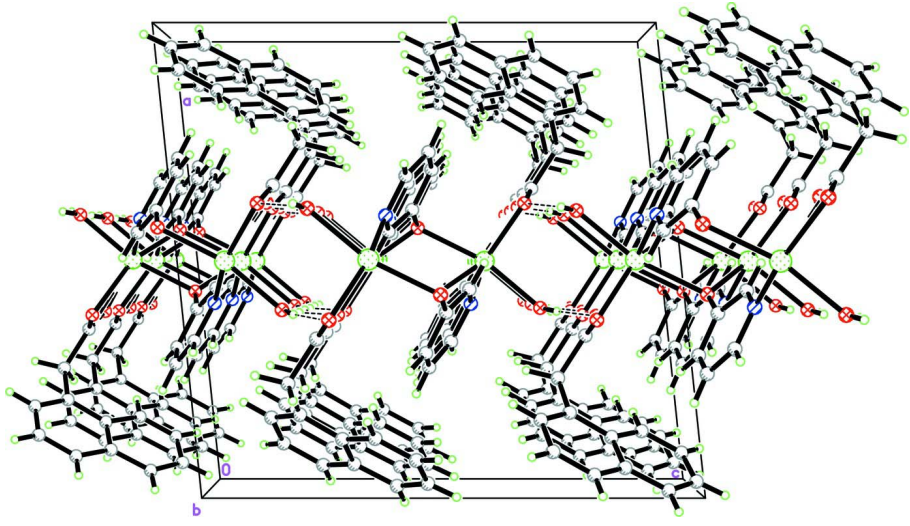


Figure 2

A packing view of the title compound. The intermolecluar hydrogen bonds are shown as dashed lines.

Poly[[aqua(1-naphthylacetato)cadmium(II)]-μ_3-pyridin-3-olato]

Crystal data

$[Cd(C_5H_4NO)(C_{12}H_9O_2)(H_2O)]$	a = 14.978 (2) Å
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Hall symbol: -P 2ybc	β = 95.928 (1)°

V = 1577.6 (3) Å^3
Z = 4
F(000) = 816
D_x = 1.725 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3600 reflections

θ = 1.4–28.0°
μ = 1.40 mm^{-1}
T = 296 K
Block, colorless
0.26 × 0.23 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.702, T_{max} = 0.757

16642 measured reflections
3617 independent reflections
3172 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −19→19
k = −8→8
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.066
S = 1.05
3617 reflections
214 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.9831P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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}
C1	0.34909 (17)	0.9822 (4)	0.28171 (15)	0.0352 (5)
C2	0.26353 (19)	0.9927 (5)	0.22167 (19)	0.0473 (7)
H2A	0.2339	1.1180	0.2305	0.057*
H2B	0.2789	0.9909	0.1632	0.057*
C3	0.19905 (18)	0.8260 (4)	0.23315 (17)	0.0443 (6)
C4	0.1889 (2)	0.6728 (6)	0.1757 (2)	0.0636 (9)
H4	0.2194	0.6762	0.1272	0.076*
C5	0.1329 (3)	0.5102 (7)	0.1888 (3)	0.0839 (13)
H5	0.1263	0.4091	0.1484	0.101*
C6	0.0885 (3)	0.4986 (7)	0.2594 (3)	0.0826 (13)

H6	0.0526	0.3890	0.2677	0.099*
C7	0.0967 (2)	0.6536 (6)	0.3206 (2)	0.0606 (9)
C8	0.0526 (2)	0.6468 (8)	0.3968 (3)	0.0859 (15)
H8	0.0160	0.5394	0.4069	0.103*
C9	0.0640 (3)	0.7988 (9)	0.4553 (3)	0.0905 (15)
H9	0.0370	0.7910	0.5058	0.109*
C10	0.1148 (3)	0.9617 (8)	0.4398 (3)	0.0819 (13)
H10	0.1197	1.0653	0.4791	0.098*
C11	0.1578 (2)	0.9751 (6)	0.3689 (2)	0.0574 (8)
H11	0.1923	1.0868	0.3602	0.069*
C12	0.15083 (17)	0.8184 (5)	0.30670 (18)	0.0453 (7)
C13	0.39701 (15)	0.6800 (3)	0.52212 (14)	0.0283 (5)
C14	0.31557 (17)	0.6297 (4)	0.47649 (16)	0.0375 (6)
H14	0.2826	0.7252	0.4441	0.045*
C15	0.28404 (19)	0.4379 (4)	0.47949 (19)	0.0443 (7)
H15	0.2294	0.4039	0.4496	0.053*
C16	0.33343 (17)	0.2974 (4)	0.52667 (17)	0.0390 (6)
H16	0.3123	0.1675	0.5272	0.047*
C17	0.44164 (16)	0.5292 (3)	0.57099 (15)	0.0294 (5)
H17	0.4948	0.5605	0.6042	0.035*
Cd1	0.501556 (11)	0.93285 (2)	0.390115 (10)	0.03064 (7)
H1W	0.608 (2)	1.071 (5)	0.266 (2)	0.046*
H2W	0.606 (2)	0.888 (5)	0.259 (2)	0.046*
N1	0.41152 (13)	0.3429 (3)	0.57215 (13)	0.0322 (4)
O1	0.38196 (12)	0.8145 (3)	0.30183 (11)	0.0405 (4)
O2	0.38678 (13)	1.1377 (3)	0.31050 (12)	0.0461 (5)
O3	0.43274 (12)	0.8600 (2)	0.51500 (10)	0.0336 (4)
O1W	0.59985 (17)	0.9759 (3)	0.28914 (15)	0.0538 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0388 (13)	0.0376 (14)	0.0295 (12)	−0.0037 (11)	0.0055 (10)	0.0013 (10)
C2	0.0433 (16)	0.0557 (17)	0.0421 (15)	−0.0011 (14)	0.0006 (12)	0.0119 (13)
C3	0.0384 (14)	0.0509 (17)	0.0413 (14)	0.0002 (12)	−0.0062 (11)	0.0040 (13)
C4	0.059 (2)	0.074 (2)	0.0542 (19)	−0.0033 (18)	−0.0098 (15)	−0.0115 (18)
C5	0.084 (3)	0.067 (3)	0.091 (3)	−0.006 (2)	−0.034 (2)	−0.020 (2)
C6	0.058 (2)	0.069 (3)	0.113 (4)	−0.020 (2)	−0.028 (2)	0.024 (3)
C7	0.0343 (15)	0.066 (2)	0.078 (2)	0.0005 (15)	−0.0060 (14)	0.0297 (19)
C8	0.046 (2)	0.098 (3)	0.114 (4)	0.005 (2)	0.010 (2)	0.061 (3)
C9	0.070 (3)	0.120 (4)	0.086 (3)	0.035 (3)	0.029 (2)	0.033 (3)
C10	0.076 (3)	0.107 (4)	0.066 (2)	0.041 (3)	0.023 (2)	0.007 (2)
C11	0.0521 (18)	0.066 (2)	0.0543 (18)	0.0172 (16)	0.0045 (14)	0.0037 (16)
C12	0.0305 (13)	0.0558 (18)	0.0483 (15)	0.0071 (12)	−0.0029 (11)	0.0138 (14)
C13	0.0357 (12)	0.0211 (11)	0.0292 (11)	0.0019 (9)	0.0077 (9)	−0.0005 (9)
C14	0.0401 (14)	0.0289 (12)	0.0424 (14)	0.0044 (11)	−0.0017 (11)	0.0044 (11)
C15	0.0377 (14)	0.0361 (15)	0.0565 (17)	−0.0050 (11)	−0.0071 (12)	0.0001 (12)
C16	0.0413 (14)	0.0245 (12)	0.0507 (15)	−0.0028 (11)	0.0024 (11)	−0.0003 (11)

C17	0.0320 (12)	0.0282 (12)	0.0279 (11)	0.0010 (9)	0.0024 (9)	−0.0002 (9)
Cd1	0.03952 (11)	0.02275 (10)	0.02918 (10)	0.00089 (7)	0.00128 (7)	0.00151 (7)
N1	0.0343 (10)	0.0251 (10)	0.0377 (11)	0.0015 (8)	0.0070 (8)	0.0028 (8)
O1	0.0458 (10)	0.0308 (10)	0.0429 (10)	−0.0008 (8)	−0.0043 (8)	−0.0026 (8)
O2	0.0555 (12)	0.0311 (10)	0.0503 (11)	−0.0001 (9)	−0.0017 (9)	0.0001 (9)
O3	0.0463 (10)	0.0218 (8)	0.0331 (8)	−0.0039 (7)	0.0058 (7)	0.0011 (7)
O1W	0.0822 (16)	0.0294 (11)	0.0547 (14)	−0.0012 (11)	0.0306 (12)	0.0036 (9)

Geometric parameters (Å, º)

C1—O2	1.252 (3)	C11—H11	0.9300
C1—O1	1.259 (3)	C13—O3	1.334 (3)
C1—C2	1.513 (4)	C13—C14	1.392 (3)
C2—C3	1.504 (4)	C13—C17	1.401 (3)
C2—H2A	0.9700	C14—C15	1.377 (4)
C2—H2B	0.9700	C14—H14	0.9300
C3—C4	1.369 (4)	C15—C16	1.371 (4)
C3—C12	1.427 (4)	C15—H15	0.9300
C4—C5	1.406 (6)	C16—N1	1.342 (3)
C4—H4	0.9300	C16—H16	0.9300
C5—C6	1.355 (6)	C17—N1	1.334 (3)
C5—H5	0.9300	C17—H17	0.9300
C6—C7	1.416 (6)	Cd1—O3^{i}	2.1992 (17)
C6—H6	0.9300	Cd1—O1	2.2931 (17)
C7—C12	1.405 (4)	Cd1—O1W	2.293 (2)
C7—C8	1.428 (6)	Cd1—N1^{ii}	2.310 (2)
C8—C9	1.375 (7)	Cd1—O3	2.3620 (16)
C8—H8	0.9300	Cd1—O2	2.4455 (19)
C9—C10	1.371 (7)	N1—Cd1^{ii}	2.310 (2)
C9—H9	0.9300	O3—Cd1^{i}	2.1992 (17)
C10—C11	1.347 (5)	O1W—H1W	0.75 (3)
C10—H10	0.9300	O1W—H2W	0.77 (3)
C11—C12	1.435 (5)		

O2—C1—O1	120.6 (2)	O3—C13—C17	122.1 (2)
O2—C1—C2	120.5 (3)	C14—C13—C17	116.7 (2)
O1—C1—C2	118.9 (2)	C15—C14—C13	119.7 (2)
C3—C2—C1	113.8 (2)	C15—C14—H14	120.1
C3—C2—H2A	108.8	C13—C14—H14	120.1
C1—C2—H2A	108.8	C16—C15—C14	119.9 (2)
C3—C2—H2B	108.8	C16—C15—H15	120.1
C1—C2—H2B	108.8	C14—C15—H15	120.1
H2A—C2—H2B	107.7	N1—C16—C15	121.5 (2)
C4—C3—C12	118.5 (3)	N1—C16—H16	119.2
C4—C3—C2	120.8 (3)	C15—C16—H16	119.2
C12—C3—C2	120.6 (3)	N1—C17—C13	123.1 (2)
C3—C4—C5	121.2 (4)	N1—C17—H17	118.4
C3—C4—H4	119.4	C13—C17—H17	118.4

C5—C4—H4	119.4	O3^{i}—Cd1—O1	153.91 (7)
C6—C5—C4	121.0 (4)	O3^{i}—Cd1—O1W	96.64 (8)
C6—C5—H5	119.5	O1—Cd1—O1W	98.15 (8)
C4—C5—H5	119.5	O3^{i}—Cd1—N1^{ii}	97.72 (7)
C5—C6—C7	119.9 (4)	O1—Cd1—N1^{ii}	105.11 (7)
C5—C6—H6	120.0	O1W—Cd1—N1^{ii}	83.93 (8)
C7—C6—H6	120.0	O3^{i}—Cd1—O3	76.72 (7)
C12—C7—C6	119.1 (3)	O1—Cd1—O3	92.91 (6)
C12—C7—C8	118.8 (4)	O1W—Cd1—O3	165.66 (8)
C6—C7—C8	122.1 (4)	N1^{ii}—Cd1—O3	84.39 (6)
C9—C8—C7	120.1 (4)	O3^{i}—Cd1—O2	103.39 (7)
C9—C8—H8	120.0	O1—Cd1—O2	54.69 (6)
C7—C8—H8	120.0	O1W—Cd1—O2	92.40 (8)
C10—C9—C8	120.7 (4)	N1^{ii}—Cd1—O2	158.86 (7)
C10—C9—H9	119.7	O3—Cd1—O2	101.47 (6)
C8—C9—H9	119.7	C17—N1—C16	119.0 (2)
C11—C10—C9	121.5 (5)	C17—N1—Cd1^{ii}	125.24 (16)
C11—C10—H10	119.3	C16—N1—Cd1^{ii}	112.99 (16)
C9—C10—H10	119.3	C1—O1—Cd1	95.81 (15)
C10—C11—C12	120.5 (4)	C1—O2—Cd1	88.89 (16)
C10—C11—H11	119.8	C13—O3—Cd1^{i}	132.39 (14)
C12—C11—H11	119.8	C13—O3—Cd1	118.14 (14)
C7—C12—C3	120.2 (3)	Cd1^{i}—O3—Cd1	103.28 (7)
C7—C12—C11	118.5 (3)	Cd1—O1W—H1W	126 (3)
C3—C12—C11	121.3 (3)	Cd1—O1W—H2W	117 (2)
O3—C13—C14	121.0 (2)	H1W—O1W—H2W	109 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*···O1^{iii}	0.75 (3)	1.97 (3)	2.720 (3)	174 (4)
O1*W*—H2*W*···O2^{iv}	0.77 (3)	2.02 (3)	2.783 (3)	173 (3)

Symmetry codes: (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) −*x*+1, *y*−1/2, −*z*+1/2.