

Poly[*diaquabis(nitrato-κ²O,O')*bis(1,10-phenanthroline-κ²N,N')-μ₃-succinato-dicadmium]

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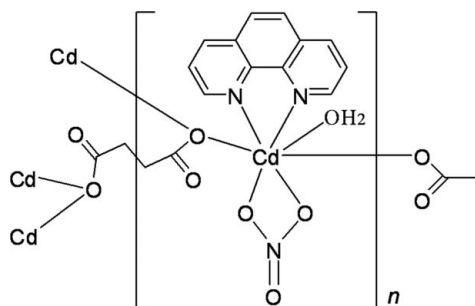
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Key indicators: single-crystal X-ray study; $T = 110$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.026; wR factor = 0.086; data-to-parameter ratio = 11.7.

In the title coordination polymer, $[\text{Cd}_2(\text{C}_4\text{H}_4\text{O}_4)(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]_n$, the Cd^{II} ion is seven-coordinated within a distorted pentagonal-bipyramidal O_5N_2 environment. The succinate anions, located on an inversion centre, adopt a bimonodentate bridging mode, leading to the formation of rods along [100]. The rods are connected by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the coordinating water molecules and nitrate O atoms of adjacent rods; the same type of hydrogen bonds are also observed between water and carboxylate O atoms within the rods. $\pi-\pi$ stacking interactions with a minimum plane-to-plane separation of $3.462(2)$ Å occur between phenanthroline ligands.

Related literature

For the structures and properties of other cadmium coordination compounds, see: Montney *et al.* (2007); Li *et al.* (2011).



Experimental

Crystal data

$[\text{Cd}_2(\text{C}_4\text{H}_4\text{O}_4)(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$	$\beta = 106.059(2)^\circ$
$M_r = 861.33$	$\gamma = 107.003(2)^\circ$
Triclinic, $P\bar{1}$	$V = 713.0(2)$ Å ³
$a = 7.7349(13)$ Å	$Z = 1$
$b = 9.4467(16)$ Å	Mo $K\alpha$ radiation
$c = 11.2063(18)$ Å	$\mu = 1.57$ mm ⁻¹
$\alpha = 102.284(2)^\circ$	$T = 110$ K
	$0.40 \times 0.34 \times 0.32$ mm

Data collection

Bruker APEXII CCD diffractometer	5357 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2008)	2617 independent reflections
$T_{\text{min}} = 0.572$, $T_{\text{max}} = 0.633$	2333 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.086$	$\Delta\rho_{\text{max}} = 0.82$ e Å ⁻³
$S = 1.10$	$\Delta\rho_{\text{min}} = -0.74$ e Å ⁻³
2617 reflections	
223 parameters	
2 restraints	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H1B}\cdots\text{O3}^{\text{i}}$	0.86 (1)	1.93 (1)	2.786 (5)	174 (5)
$\text{O1W}-\text{H1A}\cdots\text{O2}^{\text{ii}}$	0.86 (1)	1.88 (2)	2.716 (4)	166 (5)

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2640).

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supporting information

Acta Cryst. (2012). E68, m899 [https://doi.org/10.1107/S1600536812025287]

Poly[*diaquabis(nitrato-κ²O,O')*bis(1,10-phenanthroline-κ²N,N')-μ₃-succinato-dicadmium]

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S1. Comment

Cadmium(II) coordination compounds have been increasingly studied owing to their interesting physical and chemical properties (Montney *et al.*, 2007; Li *et al.*, 2011). In order to extend our knowledge in this field, we investigated the structure of the cadmium(II) title compound, [Cd₂(C₄H₄O₄)(H₂O)₂(C₁₂H₈N₂)₂(NO₃)₂], (I).

The asymmetric unit of (I) (Fig. 1) contains one Cd^{II} ion, half of a succinate anion, one nitrate anion, one coordinating water and one 1,10-phenanthroline ligand. The Cd^{II} cation is seven-coordinated by five O atoms from two succinate anions, one water molecule and a chelating nitrate anion, and two N atoms from a 1,10-phenanthroline molecule. The coordination geometry around Cd^{II} might be described as a distorted pentagonal bipyramid. The succinate anions adopt a bis-monodentate bridging coordination mode, generating rods along [100]. Adjacent rods are connected by O—H⋯O hydrogen bonds and aromatic π—π stacking interactions [minimum plane-to-plane separation of 3.462 (2) Å] to generate a three-dimensional network (Figs. 2,3).

The Cd—N and Cd—O bond lengths are 2.358 (4)–2.360 (4) Å and 2.253 (3)–2.511 (3) Å, respectively, which are comparable to those reported for other Cd(II)—O and Cd(II)—N donor complexes (Montney *et al.*, 2007; Li *et al.*, 2011).

S2. Experimental

A mixture of Cd(NO₃)₂·4H₂O (0.155 g, 0.50 mmol), succinic acid (0.029 g, 0.25 mmol), 1,10-phenanthroline (0.10 g, 0.5 mmol), NaOH (0.02 g, 0.5 mmol), and water (10 ml) was stirred at room temperature for 15 min, and then sealed in a 25 ml Teflon-lined, stainless-steel Parr bomb. The bomb was heated at 433 K for 3 days. Upon cooling, the solution yielded single crystals of the title complex in *ca* 65% yield. Anal. Calcd for C₁₄H₁₂N₃O₆Cd: C, 39.04; H, 2.81; N, 9.76. Found: C, 38.73; H, 3.14; N, 9.63.

S3. Refinement

The coordinating water H atoms were located in a different Fourier map and refined with distance constraints of O—H = 0.83 (3) Å. The carbon-bound H atoms were placed in geometrically idealized positions, with C—H = 0.93 Å, and constrained to ride on their respective parent atoms, with *U*_{iso}(H) = 1.2 *U*_{eq}(C).

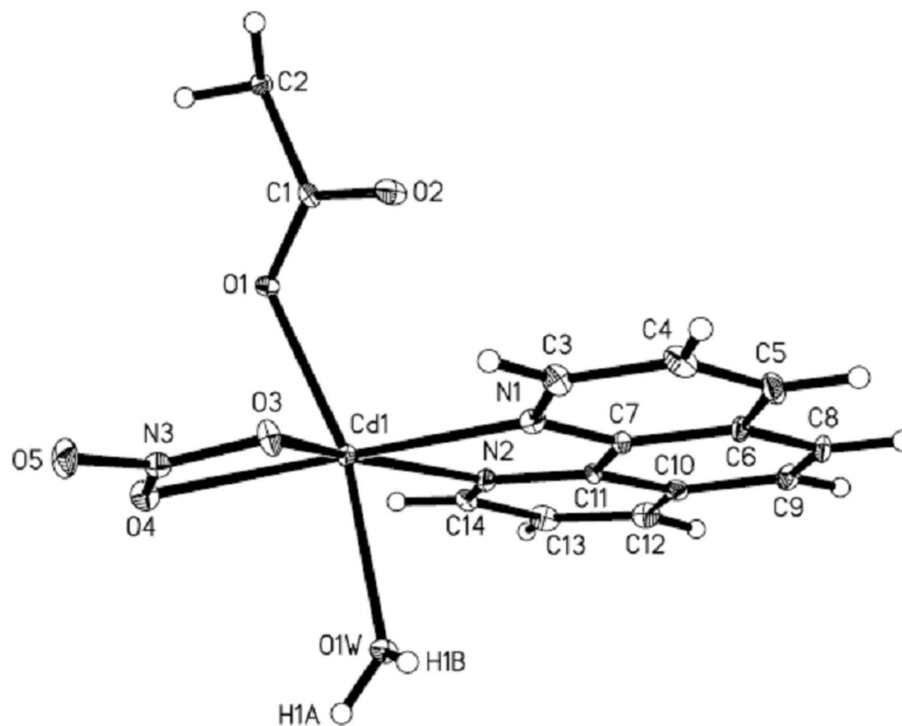


Figure 1

The asymmetric unit of the structure of (I) with displacement ellipsoids drawn at the 30% probability level.

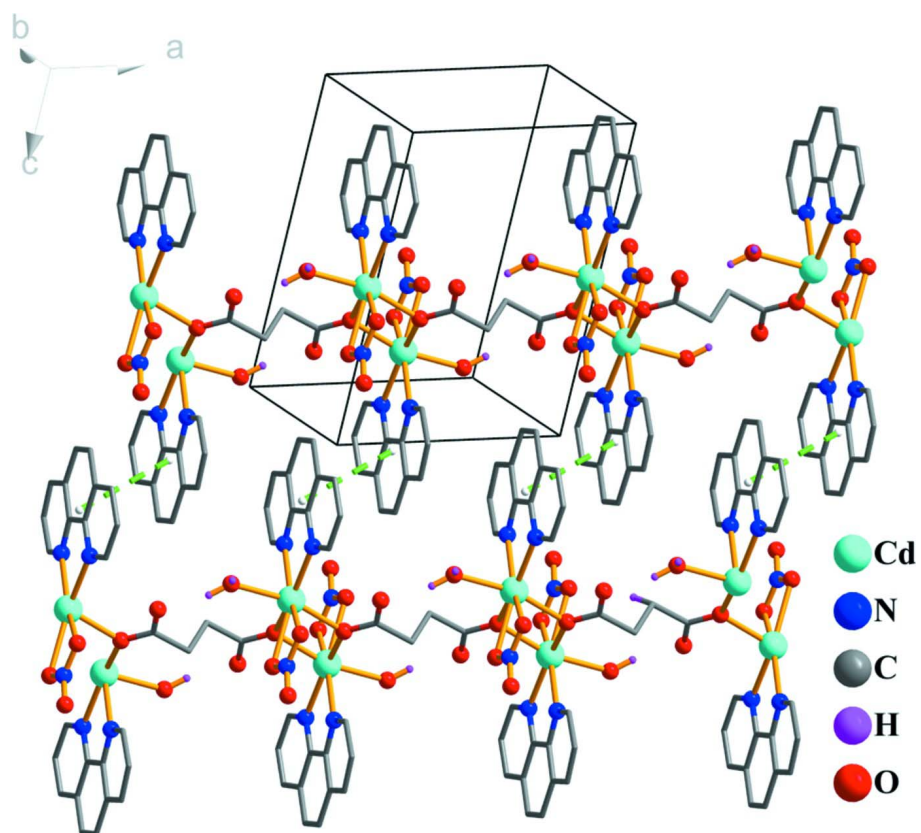


Figure 2

View approximately along the *b* axis, showing the rods parallel to [100] in the title complex. The green dashed lines represent π - π stacking interactions.

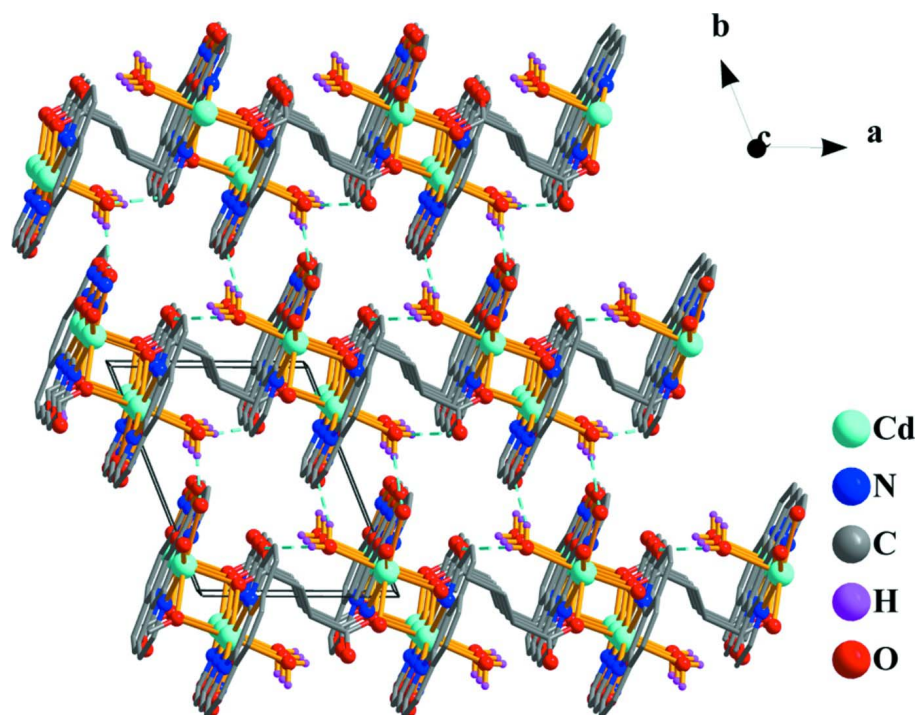


Figure 3

View along the *c* axis, showing the three-dimensional supramolecular network. Blue dashed lines represent O—H···O hydrogen bonds.

Poly[di aquabis(nitrato- κ^2 O, O')bis(1,10-phenanthroline- κ^2 N, N')- μ_3 -succinato-dicadmium]

Crystal data

$[\text{Cd}_2(\text{C}_4\text{H}_4\text{O}_4)(\text{NO}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2]$

$M_r = 861.33$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 7.7349$ (13) Å

$b = 9.4467$ (16) Å

$c = 11.2063$ (18) Å

$\alpha = 102.284$ (2)°

$\beta = 106.059$ (2)°

$\gamma = 107.003$ (2)°

$V = 713.0$ (2) Å³

$Z = 1$

$F(000) = 426$

$D_x = 2.006$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4041 reflections

$\theta = 2.4\text{--}25.5^\circ$

$\mu = 1.57$ mm⁻¹

$T = 110$ K

Block, colorless

$0.40 \times 0.34 \times 0.32$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.572$, $T_{\max} = 0.633$

5357 measured reflections

2617 independent reflections

2333 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.0^\circ$

$h = -9 \rightarrow 9$

$k = -11 \rightarrow 11$

$l = -13 \rightarrow 13$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.026$ $wR(F^2) = 0.086$ $S = 1.10$

2617 reflections

223 parameters

2 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sitesH atoms treated by a mixture of independent
and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 3.2233P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.82 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$ *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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.04544 (4)	0.84510 (4)	0.07477 (3)	0.01071 (12)
N2	0.2174 (5)	1.0166 (4)	0.2915 (4)	0.0132 (8)
N1	-0.0501 (5)	0.7203 (4)	0.2200 (4)	0.0142 (8)
C5	-0.1372 (7)	0.5878 (6)	0.4074 (5)	0.0177 (10)
H5	-0.1662	0.5412	0.4702	0.021*
C14	0.3403 (6)	1.1629 (5)	0.3271 (4)	0.0153 (9)
H14	0.3565	1.2070	0.2604	0.018*
C3	-0.1898 (7)	0.5807 (5)	0.1841 (5)	0.0174 (10)
H3	-0.2601	0.5262	0.0933	0.021*
C13	0.4480 (7)	1.2563 (5)	0.4588 (5)	0.0178 (10)
H13	0.5356	1.3604	0.4803	0.021*
C6	0.0091 (7)	0.7368 (6)	0.4475 (4)	0.0155 (9)
C7	0.0472 (6)	0.7983 (5)	0.3497 (4)	0.0123 (9)
C11	0.1893 (6)	0.9555 (5)	0.3877 (4)	0.0131 (9)
C8	0.1133 (7)	0.8288 (6)	0.5828 (4)	0.0180 (10)
H8	0.0885	0.7863	0.6487	0.022*
C9	0.2449 (7)	0.9734 (6)	0.6180 (5)	0.0200 (10)
H9	0.3107	1.0318	0.7084	0.024*
C10	0.2890 (6)	1.0423 (5)	0.5221 (4)	0.0141 (9)
C12	0.4230 (7)	1.1927 (5)	0.5559 (5)	0.0187 (10)
H12	0.4973	1.2515	0.6454	0.022*
C4	-0.2371 (7)	0.5112 (6)	0.2757 (5)	0.0197 (10)
H4	-0.3380	0.4114	0.2467	0.024*
O1W	0.2864 (5)	0.7375 (4)	0.1138 (3)	0.0147 (7)

O4	0.0112 (4)	0.7484 (4)	-0.1567 (3)	0.0166 (7)
O3	-0.1556 (5)	0.5788 (4)	-0.0899 (3)	0.0193 (7)
N3	-0.1132 (5)	0.6148 (4)	-0.1844 (4)	0.0129 (8)
O5	-0.1930 (5)	0.5236 (4)	-0.2976 (3)	0.0226 (8)
O1	-0.1906 (4)	0.9255 (4)	-0.0170 (3)	0.0141 (6)
O2	-0.3962 (5)	0.7674 (4)	0.0468 (3)	0.0204 (7)
C1	-0.3553 (6)	0.8680 (5)	-0.0059 (4)	0.0103 (8)
C2	-0.5043 (6)	0.9368 (5)	-0.0573 (4)	0.0118 (9)
H2A	-0.6357	0.8539	-0.0978	0.014*
H2B	-0.4758	0.9823	-0.1247	0.014*
H1B	0.238 (7)	0.6402 (19)	0.106 (5)	0.018*
H1A	0.373 (5)	0.736 (6)	0.080 (5)	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01089 (18)	0.01093 (18)	0.00981 (18)	0.00348 (12)	0.00347 (12)	0.00352 (12)
N2	0.0124 (18)	0.016 (2)	0.0127 (18)	0.0055 (16)	0.0053 (15)	0.0070 (15)
N1	0.0144 (19)	0.0113 (19)	0.0161 (19)	0.0050 (15)	0.0048 (15)	0.0032 (15)
C5	0.023 (3)	0.019 (2)	0.020 (2)	0.010 (2)	0.014 (2)	0.012 (2)
C14	0.014 (2)	0.020 (2)	0.015 (2)	0.0075 (19)	0.0068 (18)	0.0064 (18)
C3	0.019 (2)	0.012 (2)	0.019 (2)	0.0028 (19)	0.0079 (19)	0.0040 (18)
C13	0.015 (2)	0.007 (2)	0.026 (3)	-0.0007 (18)	0.008 (2)	0.0010 (19)
C6	0.020 (2)	0.021 (2)	0.016 (2)	0.013 (2)	0.0106 (19)	0.0131 (19)
C7	0.011 (2)	0.015 (2)	0.014 (2)	0.0058 (18)	0.0053 (17)	0.0076 (18)
C11	0.015 (2)	0.020 (2)	0.011 (2)	0.0110 (19)	0.0081 (17)	0.0057 (18)
C8	0.023 (2)	0.027 (3)	0.013 (2)	0.014 (2)	0.0093 (19)	0.012 (2)
C9	0.020 (2)	0.027 (3)	0.014 (2)	0.011 (2)	0.0046 (19)	0.006 (2)
C10	0.015 (2)	0.014 (2)	0.014 (2)	0.0082 (18)	0.0056 (18)	0.0013 (18)
C12	0.016 (2)	0.015 (2)	0.018 (2)	0.0037 (19)	0.0029 (19)	-0.0013 (19)
C4	0.019 (2)	0.017 (2)	0.023 (3)	0.006 (2)	0.011 (2)	0.003 (2)
O1W	0.0139 (16)	0.0115 (16)	0.0203 (17)	0.0042 (13)	0.0083 (13)	0.0062 (13)
O4	0.0154 (16)	0.0109 (16)	0.0195 (17)	-0.0002 (13)	0.0063 (13)	0.0044 (13)
O3	0.0243 (18)	0.0210 (18)	0.0138 (16)	0.0057 (15)	0.0113 (14)	0.0062 (14)
N3	0.0138 (19)	0.0103 (19)	0.0136 (19)	0.0047 (15)	0.0048 (15)	0.0019 (15)
O5	0.0228 (18)	0.0244 (19)	0.0096 (16)	0.0025 (15)	0.0019 (14)	-0.0015 (14)
O1	0.0081 (15)	0.0195 (17)	0.0137 (15)	0.0036 (13)	0.0037 (12)	0.0057 (13)
O2	0.0181 (17)	0.0206 (18)	0.036 (2)	0.0104 (14)	0.0169 (15)	0.0219 (16)
C1	0.015 (2)	0.006 (2)	0.011 (2)	0.0038 (17)	0.0065 (17)	0.0012 (16)
C2	0.011 (2)	0.011 (2)	0.015 (2)	0.0026 (17)	0.0047 (17)	0.0082 (18)

Geometric parameters (Å, °)

Cd1—O1	2.253 (3)	C7—C11	1.453 (6)
Cd1—O1W	2.355 (3)	C11—C10	1.414 (6)
Cd1—N1	2.358 (4)	C8—C9	1.340 (7)
Cd1—N2	2.360 (4)	C8—H8	0.9500
Cd1—O1 ⁱ	2.439 (3)	C9—C10	1.437 (7)

Cd1—O4	2.470 (3)	C9—H9	0.9500
Cd1—O3	2.511 (3)	C10—C12	1.389 (7)
N2—C14	1.327 (6)	C12—H12	0.9500
N2—C11	1.365 (6)	C4—H4	0.9500
N1—C3	1.330 (6)	O1W—H1B	0.859 (10)
N1—C7	1.355 (6)	O1W—H1A	0.859 (10)
C5—C4	1.374 (7)	O4—N3	1.254 (5)
C5—C6	1.407 (7)	O3—N3	1.275 (5)
C5—H5	0.9500	N3—O5	1.234 (5)
C14—C13	1.410 (6)	O1—C1	1.282 (5)
C14—H14	0.9500	O1—Cd1 ⁱ	2.439 (3)
C3—C4	1.405 (7)	O2—C1	1.232 (5)
C3—H3	0.9500	C1—C2	1.521 (6)
C13—C12	1.381 (7)	C2—C2 ⁱⁱ	1.528 (9)
C13—H13	0.9500	C2—H2A	0.9900
C6—C7	1.406 (6)	C2—H2B	0.9900
C6—C8	1.435 (7)		
O1—Cd1—O1W	165.04 (11)	N1—C7—C6	122.8 (4)
O1—Cd1—N1	107.49 (12)	N1—C7—C11	117.9 (4)
O1W—Cd1—N1	83.07 (12)	C6—C7—C11	119.3 (4)
O1—Cd1—N2	107.06 (12)	N2—C11—C10	122.0 (4)
O1W—Cd1—N2	86.20 (12)	N2—C11—C7	118.5 (4)
N1—Cd1—N2	70.97 (13)	C10—C11—C7	119.4 (4)
O1—Cd1—O1 ⁱ	71.54 (12)	C9—C8—C6	121.2 (4)
O1W—Cd1—O1 ⁱ	103.94 (10)	C9—C8—H8	119.4
N1—Cd1—O1 ⁱ	153.21 (12)	C6—C8—H8	119.4
N2—Cd1—O1 ⁱ	83.58 (11)	C8—C9—C10	121.5 (4)
O1—Cd1—O4	81.10 (11)	C8—C9—H9	119.2
O1W—Cd1—O4	83.94 (11)	C10—C9—H9	119.2
N1—Cd1—O4	133.14 (12)	C12—C10—C11	118.3 (4)
N2—Cd1—O4	152.10 (12)	C12—C10—C9	122.7 (4)
O1 ⁱ —Cd1—O4	73.64 (10)	C11—C10—C9	119.0 (4)
O1—Cd1—O3	87.96 (11)	C13—C12—C10	119.8 (4)
O1W—Cd1—O3	82.85 (11)	C13—C12—H12	120.1
N1—Cd1—O3	82.58 (12)	C10—C12—H12	120.1
N2—Cd1—O3	152.40 (12)	C5—C4—C3	119.9 (4)
O1 ⁱ —Cd1—O3	123.65 (10)	C5—C4—H4	120.1
O4—Cd1—O3	51.17 (10)	C3—C4—H4	120.1
C14—N2—C11	118.1 (4)	Cd1—O1W—H1B	112 (4)
C14—N2—Cd1	126.2 (3)	Cd1—O1W—H1A	132 (4)
C11—N2—Cd1	115.7 (3)	H1B—O1W—H1A	99 (5)
C3—N1—C7	118.5 (4)	N3—O4—Cd1	97.2 (2)
C3—N1—Cd1	125.0 (3)	N3—O3—Cd1	94.7 (2)
C7—N1—Cd1	116.5 (3)	O5—N3—O4	121.9 (4)
C4—C5—C6	118.8 (4)	O5—N3—O3	121.5 (4)
C4—C5—H5	120.6	O4—N3—O3	116.6 (3)
C6—C5—H5	120.6	C1—O1—Cd1	117.6 (3)

N2—C14—C13	123.4 (4)	C1—O1—Cd1 ⁱ	132.2 (3)
N2—C14—H14	118.3	Cd1—O1—Cd1 ⁱ	108.46 (12)
C13—C14—H14	118.3	O2—C1—O1	124.8 (4)
N1—C3—C4	122.3 (4)	O2—C1—C2	119.1 (4)
N1—C3—H3	118.9	O1—C1—C2	116.0 (4)
C4—C3—H3	118.9	C1—C2—C2 ⁱⁱ	108.6 (4)
C12—C13—C14	118.3 (4)	C1—C2—H2A	110.0
C12—C13—H13	120.8	C2 ⁱⁱ —C2—H2A	110.0
C14—C13—H13	120.8	C1—C2—H2B	110.0
C7—C6—C5	117.9 (4)	C2 ⁱⁱ —C2—H2B	110.0
C7—C6—C8	119.6 (4)	H2A—C2—H2B	108.4
C5—C6—C8	122.5 (4)		
O1—Cd1—N2—C14	-73.4 (4)	C5—C6—C8—C9	-176.6 (5)
O1W—Cd1—N2—C14	99.5 (4)	C6—C8—C9—C10	-0.6 (7)
N1—Cd1—N2—C14	-176.5 (4)	N2—C11—C10—C12	-1.8 (6)
O1 ⁱ —Cd1—N2—C14	-5.0 (3)	C7—C11—C10—C12	-179.5 (4)
O4—Cd1—N2—C14	30.1 (5)	N2—C11—C10—C9	176.9 (4)
O3—Cd1—N2—C14	166.2 (3)	C7—C11—C10—C9	-0.9 (6)
O1—Cd1—N2—C11	108.4 (3)	C8—C9—C10—C12	179.2 (4)
O1W—Cd1—N2—C11	-78.7 (3)	C8—C9—C10—C11	0.6 (7)
N1—Cd1—N2—C11	5.3 (3)	C14—C13—C12—C10	-2.4 (7)
O1 ⁱ —Cd1—N2—C11	176.8 (3)	C11—C10—C12—C13	3.5 (7)
O4—Cd1—N2—C11	-148.1 (3)	C9—C10—C12—C13	-175.1 (4)
O3—Cd1—N2—C11	-12.0 (5)	C6—C5—C4—C3	1.2 (7)
O1—Cd1—N1—C3	72.5 (4)	N1—C3—C4—C5	-0.1 (7)
O1W—Cd1—N1—C3	-96.7 (4)	O1—Cd1—O4—N3	-91.1 (2)
N2—Cd1—N1—C3	175.0 (4)	O1W—Cd1—O4—N3	89.2 (2)
O1 ⁱ —Cd1—N1—C3	156.0 (3)	N1—Cd1—O4—N3	14.6 (3)
O4—Cd1—N1—C3	-21.7 (4)	N2—Cd1—O4—N3	159.1 (3)
O3—Cd1—N1—C3	-13.0 (4)	O1 ⁱ —Cd1—O4—N3	-164.3 (3)
O1—Cd1—N1—C7	-107.8 (3)	O3—Cd1—O4—N3	3.5 (2)
O1W—Cd1—N1—C7	83.1 (3)	O1—Cd1—O3—N3	76.8 (2)
N2—Cd1—N1—C7	-5.3 (3)	O1W—Cd1—O3—N3	-91.4 (2)
O1 ⁱ —Cd1—N1—C7	-24.3 (5)	N1—Cd1—O3—N3	-175.3 (3)
O4—Cd1—N1—C7	158.0 (3)	N2—Cd1—O3—N3	-158.8 (3)
O3—Cd1—N1—C7	166.7 (3)	O1 ⁱ —Cd1—O3—N3	10.6 (3)
C11—N2—C14—C13	2.3 (6)	O4—Cd1—O3—N3	-3.4 (2)
Cd1—N2—C14—C13	-175.8 (3)	Cd1—O4—N3—O5	172.9 (3)
C7—N1—C3—C4	-1.1 (7)	Cd1—O4—N3—O3	-6.0 (4)
Cd1—N1—C3—C4	178.6 (3)	Cd1—O3—N3—O5	-173.1 (3)
N2—C14—C13—C12	-0.6 (7)	Cd1—O3—N3—O4	5.9 (4)
C4—C5—C6—C7	-1.0 (7)	O1W—Cd1—O1—C1	118.5 (4)
C4—C5—C6—C8	176.5 (4)	N1—Cd1—O1—C1	-15.1 (3)
C3—N1—C7—C6	1.3 (6)	N2—Cd1—O1—C1	-90.0 (3)
Cd1—N1—C7—C6	-178.5 (3)	O1 ⁱ —Cd1—O1—C1	-166.9 (4)
C3—N1—C7—C11	-175.4 (4)	O4—Cd1—O1—C1	117.4 (3)
Cd1—N1—C7—C11	4.8 (5)	O3—Cd1—O1—C1	66.4 (3)

C5—C6—C7—N1	-0.2 (7)	O1W—Cd1—O1—Cd1 ⁱ	-74.6 (4)
C8—C6—C7—N1	-177.8 (4)	N1—Cd1—O1—Cd1 ⁱ	151.83 (13)
C5—C6—C7—C11	176.4 (4)	N2—Cd1—O1—Cd1 ⁱ	76.95 (14)
C8—C6—C7—C11	-1.1 (6)	O1 ⁱ —Cd1—O1—Cd1 ⁱ	0.0
C14—N2—C11—C10	-1.1 (6)	O4—Cd1—O1—Cd1 ⁱ	-75.62 (12)
Cd1—N2—C11—C10	177.3 (3)	O3—Cd1—O1—Cd1 ⁱ	-126.61 (12)
C14—N2—C11—C7	176.7 (4)	Cd1—O1—C1—O2	-2.9 (6)
Cd1—N2—C11—C7	-5.0 (5)	Cd1 ⁱ —O1—C1—O2	-166.1 (3)
N1—C7—C11—N2	0.2 (6)	Cd1—O1—C1—C2	174.2 (3)
C6—C7—C11—N2	-176.7 (4)	Cd1 ⁱ —O1—C1—C2	11.0 (5)
N1—C7—C11—C10	178.0 (4)	O2—C1—C2—C2 ⁱⁱ	81.3 (6)
C6—C7—C11—C10	1.1 (6)	O1—C1—C2—C2 ⁱⁱ	-96.0 (5)
C7—C6—C8—C9	0.8 (7)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1B \cdots O3 ⁱⁱⁱ	0.86 (1)	1.93 (1)	2.786 (5)	174 (5)
O1W—H1A \cdots O2 ^{iv}	0.86 (1)	1.88 (2)	2.716 (4)	166 (5)

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