Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[[bis[(2,2′-bipyridine-κ^2N,N')-cadmium(II)]-bis[μ_3-3-(4-carboxylatophenoxy)propionato-$\kappa^5O,O':O':O'',O'''$]] 4-hydroxybenzoic acid monohydrate]

Li-Li Kong,[a] Shan Gao,[a] Li-Hua Huo[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

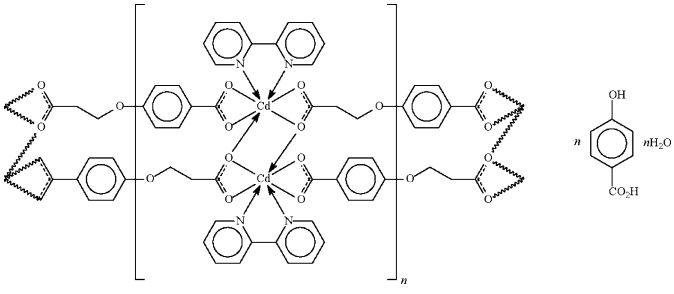
Received 23 October 2007; accepted 30 October 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.040; wR factor = 0.120; data-to-parameter ratio = 14.7.

The 3-(4-carboxylatophenoxy)propionate dianion in the title compound, $[Cd_2(C_{10}H_8O_5)_2(C_{10}H_8N_2)_2]\cdot C_7H_6O_3\cdot H_2O$, links adjacent metal atoms into a chain, the dianion chelating through both O atoms of its two $-CO_2^-$ end groups. One of the carboxylate O atoms (that belonging to the aliphatic carboxylate end) engages in interchain coordination, linking two chains into a ribbon. The ribbons are linked to the disordered water molecule and 4-hydroxybenzoic acid by O—H···O hydrogen bonds, further consolidating the ribbon motif. The Cd^{II} atom exists in a seven-coordinate CdN_2O_5 enviroment that approximates to a monocapped octahedron. The dinuclear repeat unit is centrosymmetric.

Related literature

For 2,2′-bipyridine-chelated transition metal derivatives of 3-(4-carboxylatophenoxy)propionic acid, see: Kong *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Cd_2(C_{10}H_8O_5)_2(C_{10}H_8N_2)_2]\cdot C_7H_6O_3\cdot H_2O$
M_r = 1109.63
Triclinic, $P\overline{1}$
a = 10.1615 (5) Å
b = 10.6255 (5) Å
c = 10.8507 (6) Å
α = 73.147 (2)°
β = 82.174 (1)°
γ = 88.734 (1)°
V = 1110.6 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 295 (2) K
0.32 × 0.24 × 0.16 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.542, T_{max} = 0.852
10857 measured reflections
5010 independent reflections
3997 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.120
S = 1.06
5010 reflections
341 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1	2.511 (4)	Cd1—O5^{ii}	2.370 (3)
Cd1—O2	2.345 (3)	Cd1—N1	2.339 (3)
Cd1—O2^{i}	2.406 (3)	Cd1—N2	2.323 (4)
Cd1—O4^{ii}	2.351 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7o···O1w^{iii}	0.82	1.75	2.55 (1)	166
O8—H8o···O1	0.82	2.01	2.815 (8)	168
O1w—H1w···O1^{iv}	0.82	1.98	2.797 (8)	171
O1w—H2w···O8	0.82	2.11	2.93 (1)	172

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

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001), *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

We thank the Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036), Heilongjiang University and the University of Malaya for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2610).

  doi:10.1107/S1600536807054669

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *J. Appl. Cryst.* **36**, 1283–1284.
Higashi, T. (1995). *ABSCOR*. Rigaku, Tokyo, Japan.
Kong, L.-L., Gao, S., Huo, L.-H. & Ng, S. W. (2007*a*). *Acta Cryst.* E**63**, m2851.
Kong, L.-L., Gao, S., Huo, L.-H. & Ng, S. W. (2007*b*). *Acta Cryst.* E**63**, m2852.
Rigaku Corporation (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Westrip, S. P. (2007). *publCIF*. In preparation.

supplementary materials

Acta Cryst. (2007). E**63**, m2938-m2939 [**doi:10.1107/S1600536807054669**]

Poly[[[bis[(2,2'-bipyridine-κ^2N,N')cadmium(II)]-bis[μ_3-3-(4-carboxylatophenoxy)propionato-$\kappa^5O,O':O':O'',O'''$]] 4-hydroxybenzoic acid monohydrate]

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Comment

The present study on the title compound, (I), follows reports on the transition metal derivatives of 3-(4-carboxylatophenoxy)propionic acid. These (Kong *et al.*, 2007*a*,b) describe the isostrutural manganese(II) and cobalt(II) adducts with 2,2'-bipyridine. With cadmium nitrate as reactant and by using a hydrothermal method, part of the carboxylic acid is hydrolyzed to give 4-hydroxybenzoic acid, which is then incorporated into the crystal structure (Fig. 1). Topologically, a double ribbon polyer is formed (Fig. 2).

The cadmium(II) atom in (I) exists in a seven-coordinate CdN_2O_5 enviroment (Fig. 3) that approximates to a monocapped octahedron (Table 1) and a network of O—H···O hydrogen bonds (Table 2) helps to consolidate the structure.

Experimental

Cadmium dinitrate tetrahydrate (2 mmol), 2,2'-bipyridine (2 mmol) and 3-(4-carboxylatophenoxy)propionic acid (2 mmol) and water were sealed in a 25-ml, Teflon-lined, stainless steel bomb and heated at 413 K for 20 h. The bomb was cooled to room temperature; the colorless crystals that separated was picked out manually.

Refinement

The water and 4-hydroxybenzoic acid molecules are disordered about a center-of-inversion; the molecules were assigned half-occupancy each. The phenylene ring was refined as a rigid hexagon of 1.39 Å sides. The four-atom –C(=O)–O fragment was restrained to be nearly planar; the two C–O distances were restrained to 1.25±0.01 Å and the C–C single-bond distance to 1.50±-0.01 Å.

Carbon-bound H atoms were placed in calculated positions [C—H 0.93–0.97 Å and U_{iso}(H) 1.2U_{eq}(C)], and were included in the refinement in the riding-model approximation. The carboxylic acid and water H-atoms were similarly generated [O–H 0.82 Å and and U_{iso}(H) 1.2U_{eq}(O)].

The final difference Fourier map had a large peak near Cd1, but was otherwise essentially featureless.

Figures

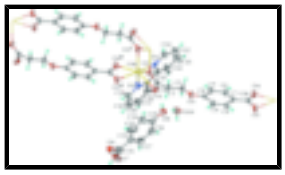


Fig. 1. **Figure 1**. View of a fragment of (I); displacement ellipsoids are drawn at the 50% probability level, and H atoms as spheres of arbitrary radius. Symmetry codes are given in Table 1.

Fig. 2. **Figure 2**. A representation of the polymeric double ribbon structure in (I).

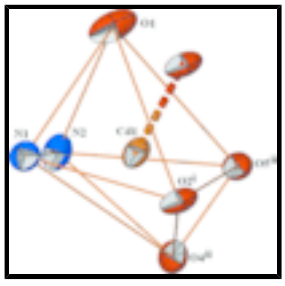


Fig. 3. **Figure 3**. Seven-coordinate geometry of cadmium in (I).

Poly[[[bis[(2,2'-bipyridine-κ^2N,N')cadmium(II)]- bis[μ_3-3-(4-carboxylatophenoxy)propionato-$\kappa^5O,O':O':O'',O'''$]] 4-hydroxybenzoic acid monohydrate]

Crystal data

$[Cd_2(C_{10}H_8O_5)_2(C_{10}H_8N_2)_2]\cdot C_7H_6O_3\cdot H_2O$	$Z = 1$
$M_r = 1109.63$	$F_{000} = 558$
Triclinic, $P\overline{1}$	$D_x = 1.659$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.1615$ (5) Å	Cell parameters from 8754 reflections
$b = 10.6255$ (5) Å	$\theta = 3.0$–27.5°
$c = 10.8507$ (6) Å	$\mu = 1.03$ mm^{-1}
$\alpha = 73.147$ (2)°	$T = 295$ (2) K
$\beta = 82.174$ (1)°	Block, colorless
$\gamma = 88.734$ (1)°	0.32 × 0.24 × 0.16 mm
$V = 1110.6$ (1) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	5010 independent reflections
Radiation source: fine-focus sealed tube	3997 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 295(2)$ K	$\theta_{min} = 3.0^\circ$
ω–scans	$h = -13\rightarrow13$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -11\rightarrow13$
$T_{min} = 0.542$, $T_{max} = 0.852$	$l = -14\rightarrow14$
10857 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 1.4148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
5010 reflections	$\Delta\rho_{max} = 1.13$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.87$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cd1	0.42672 (3)	0.67472 (3)	0.96257 (3)	0.04096 (12)	
O1	0.4806 (4)	0.6852 (4)	0.7269 (3)	0.0713 (11)	
O2	0.4891 (3)	0.5017 (3)	0.8745 (3)	0.0503 (7)	
O3	0.7194 (3)	0.5162 (4)	0.4709 (3)	0.0528 (8)	
O4	1.2813 (3)	0.7051 (3)	0.1393 (3)	0.0524 (8)	
O5	1.1998 (3)	0.6081 (3)	0.0120 (3)	0.0501 (8)	
N1	0.6322 (3)	0.7835 (4)	0.9263 (3)	0.0422 (8)	
N2	0.3986 (3)	0.8980 (4)	0.8686 (4)	0.0506 (9)	
C1	0.5078 (4)	0.5672 (5)	0.7584 (4)	0.0423 (10)	
C2	0.5637 (4)	0.5052 (6)	0.6544 (4)	0.0544 (12)	
H2A	0.4973	0.5069	0.5976	0.065*	
H2B	0.5831	0.4139	0.6948	0.065*	
C3	0.6886 (4)	0.5747 (5)	0.5741 (4)	0.0501 (11)	
H3A	0.6738	0.6681	0.5399	0.060*	
H3B	0.7606	0.5627	0.6264	0.060*	
C4	0.8339 (4)	0.5545 (4)	0.3857 (4)	0.0366 (8)	
C5	0.9291 (4)	0.6386 (5)	0.4003 (4)	0.0470 (10)	
H5	0.9163	0.6751	0.4692	0.056*	
C6	1.0433 (4)	0.6675 (5)	0.3111 (4)	0.0450 (10)	
H6	1.1087	0.7219	0.3218	0.054*	
C7	1.0620 (4)	0.6166 (4)	0.2057 (4)	0.0357 (8)	
C8	0.9646 (4)	0.5349 (4)	0.1924 (4)	0.0407 (9)	

H8	0.9758	0.4997	0.1227	0.049*	
C9	0.8502 (4)	0.5047 (5)	0.2819 (4)	0.0466 (10)	
H9	0.7846	0.4506	0.2712	0.056*	
C10	1.1891 (4)	0.6454 (4)	0.1128 (4)	0.0383 (9)	
C11	0.7459 (4)	0.7223 (5)	0.9483 (5)	0.0507 (11)	
H11	0.7436	0.6317	0.9860	0.061*	
C12	0.8668 (5)	0.7873 (6)	0.9178 (6)	0.0690 (15)	
H12	0.9449	0.7416	0.9333	0.083*	
C13	0.8693 (5)	0.9193 (6)	0.8645 (8)	0.096 (3)	
H13	0.9498	0.9657	0.8426	0.115*	
C14	0.7518 (5)	0.9853 (5)	0.8427 (7)	0.0749 (18)	
H14	0.7521	1.0764	0.8090	0.090*	
C15	0.6343 (4)	0.9139 (4)	0.8718 (4)	0.0405 (9)	
C16	0.5054 (4)	0.9786 (4)	0.8424 (4)	0.0391 (9)	
C17	0.4953 (5)	1.1124 (5)	0.7919 (5)	0.0555 (12)	
H17	0.5702	1.1667	0.7754	0.067*	
C18	0.3730 (5)	1.1661 (5)	0.7658 (6)	0.0638 (14)	
H18	0.3644	1.2565	0.7322	0.077*	
C19	0.2654 (5)	1.0838 (6)	0.7902 (6)	0.0750 (17)	
H19	0.1825	1.1169	0.7717	0.090*	
C20	0.2812 (5)	0.9547 (5)	0.8413 (6)	0.0717 (17)	
H20	0.2064	0.9001	0.8594	0.086*	
O1w	0.6482 (8)	1.1595 (8)	0.4750 (9)	0.077 (2)	0.50
H1w	0.6162	1.2113	0.4151	0.092*	0.50
H2w	0.6057	1.0901	0.4959	0.092*	0.50
O6	−0.1473 (12)	0.9220 (11)	0.5206 (16)	0.089 (4)	0.50
O7	−0.1003 (11)	1.1321 (8)	0.4495 (14)	0.078 (5)	0.50
H7O	−0.1790	1.1487	0.4448	0.117*	0.50
O8	0.4798 (7)	0.9246 (7)	0.5287 (8)	0.0657 (19)	0.50
H8O	0.4907	0.8528	0.5804	0.099*	0.50
C21	−0.0645 (10)	1.0142 (12)	0.4888 (14)	0.071 (8)	0.50
C22	0.0799 (7)	0.9884 (13)	0.4960 (19)	0.059 (6)	0.50
C23	0.1194 (8)	0.8635 (11)	0.5611 (16)	0.127 (14)	0.50
H23	0.0564	0.7964	0.5983	0.153*	0.50
C24	0.2532 (9)	0.8391 (6)	0.5707 (10)	0.074 (3)	0.50
H24	0.2796	0.7555	0.6143	0.089*	0.50
C25	0.3473 (6)	0.9395 (7)	0.5152 (8)	0.054 (2)	0.50
C26	0.3077 (8)	1.0643 (6)	0.4500 (8)	0.055 (2)	0.50
H26	0.3707	1.1315	0.4128	0.066*	0.50
C27	0.1740 (9)	1.0888 (9)	0.4404 (14)	0.066 (5)	0.50
H27	0.1476	1.1724	0.3968	0.079*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03119 (16)	0.04466 (19)	0.04179 (19)	−0.00141 (12)	0.00713 (11)	−0.00967 (14)
O1	0.081 (2)	0.080 (3)	0.040 (2)	0.030 (2)	0.0032 (17)	−0.0039 (18)
O2	0.0553 (17)	0.0601 (19)	0.0309 (16)	0.0082 (15)	0.0077 (13)	−0.0127 (14)

O3	0.0361 (15)	0.083 (2)	0.0409 (17)	−0.0108 (15)	0.0124 (12)	−0.0284 (17)
O4	0.0339 (15)	0.066 (2)	0.058 (2)	−0.0112 (15)	0.0079 (13)	−0.0255 (17)
O5	0.0414 (16)	0.064 (2)	0.0483 (18)	−0.0108 (15)	0.0130 (13)	−0.0295 (16)
N1	0.0361 (17)	0.046 (2)	0.044 (2)	0.0026 (15)	−0.0018 (14)	−0.0144 (16)
N2	0.0370 (18)	0.051 (2)	0.057 (2)	−0.0029 (17)	0.0016 (16)	−0.0078 (19)
C1	0.0290 (18)	0.063 (3)	0.035 (2)	0.0069 (19)	−0.0027 (15)	−0.015 (2)
C2	0.039 (2)	0.091 (4)	0.033 (2)	−0.005 (2)	0.0071 (17)	−0.022 (2)
C3	0.037 (2)	0.077 (3)	0.035 (2)	0.003 (2)	0.0047 (17)	−0.018 (2)
C4	0.0277 (17)	0.045 (2)	0.034 (2)	0.0036 (16)	0.0028 (14)	−0.0099 (17)
C5	0.038 (2)	0.065 (3)	0.042 (2)	0.004 (2)	0.0039 (17)	−0.025 (2)
C6	0.035 (2)	0.058 (3)	0.045 (2)	−0.0091 (19)	0.0054 (17)	−0.025 (2)
C7	0.0322 (18)	0.036 (2)	0.036 (2)	0.0016 (16)	0.0032 (15)	−0.0087 (17)
C8	0.041 (2)	0.048 (2)	0.034 (2)	−0.0034 (18)	0.0062 (16)	−0.0185 (18)
C9	0.037 (2)	0.059 (3)	0.046 (3)	−0.011 (2)	0.0058 (17)	−0.022 (2)
C10	0.0299 (18)	0.038 (2)	0.043 (2)	0.0038 (16)	0.0025 (16)	−0.0093 (18)
C11	0.043 (2)	0.046 (2)	0.060 (3)	0.006 (2)	−0.010 (2)	−0.010 (2)
C12	0.039 (2)	0.063 (3)	0.102 (5)	0.004 (2)	−0.010 (3)	−0.020 (3)
C13	0.039 (3)	0.063 (4)	0.176 (8)	−0.007 (3)	−0.012 (4)	−0.019 (4)
C14	0.047 (3)	0.040 (3)	0.126 (6)	−0.002 (2)	−0.010 (3)	−0.009 (3)
C15	0.040 (2)	0.038 (2)	0.045 (2)	0.0003 (17)	−0.0021 (17)	−0.0174 (19)
C16	0.044 (2)	0.039 (2)	0.034 (2)	0.0084 (18)	−0.0026 (16)	−0.0125 (17)
C17	0.057 (3)	0.041 (2)	0.068 (3)	0.002 (2)	−0.014 (2)	−0.013 (2)
C18	0.064 (3)	0.055 (3)	0.067 (4)	0.010 (3)	−0.018 (3)	−0.005 (3)
C19	0.051 (3)	0.074 (4)	0.084 (4)	0.017 (3)	−0.022 (3)	0.007 (3)
C20	0.042 (2)	0.055 (3)	0.104 (5)	0.003 (2)	−0.017 (3)	0.002 (3)
O1w	0.071 (5)	0.061 (5)	0.082 (6)	0.008 (5)	−0.024 (5)	0.011 (4)
O6	0.068 (6)	0.077 (8)	0.132 (12)	0.000 (6)	−0.044 (8)	−0.032 (7)
O7	0.065 (6)	0.035 (5)	0.134 (13)	0.010 (5)	−0.022 (7)	−0.021 (7)
O8	0.060 (4)	0.060 (4)	0.066 (5)	0.003 (4)	−0.008 (3)	0.000 (4)
C21	0.068 (10)	0.069 (19)	0.082 (17)	0.005 (11)	−0.027 (10)	−0.025 (13)
C22	0.059 (10)	0.065 (17)	0.053 (10)	−0.009 (10)	−0.011 (8)	−0.013 (10)
C23	0.12 (2)	0.14 (2)	0.092 (18)	−0.026 (17)	−0.050 (17)	0.025 (16)
C24	0.069 (7)	0.048 (6)	0.098 (10)	0.004 (6)	−0.035 (7)	0.000 (6)
C25	0.062 (6)	0.050 (6)	0.044 (5)	0.002 (5)	−0.007 (4)	−0.004 (5)
C26	0.060 (6)	0.044 (5)	0.056 (6)	0.003 (4)	−0.004 (5)	−0.009 (4)
C27	0.079 (11)	0.045 (8)	0.066 (9)	0.001 (7)	−0.007 (7)	−0.004 (6)

Geometric parameters (Å, °)

Cd1—O1	2.511 (4)	C9—H9	0.9300
Cd1—O2	2.345 (3)	C11—C12	1.375 (7)
Cd1—O2^{i}	2.406 (3)	C11—H11	0.9300
Cd1—O4^{ii}	2.351 (3)	C12—C13	1.353 (8)
Cd1—O5^{ii}	2.370 (3)	C12—H12	0.9300
Cd1—N1	2.339 (3)	C13—C14	1.385 (7)
Cd1—N2	2.323 (4)	C13—H13	0.9300
O1—C1	1.236 (6)	C14—C15	1.378 (6)
O2—C1	1.241 (5)	C14—H14	0.9300

O2—Cd1^{i}	2.406 (3)	C15—C16	1.496 (6)
O3—C4	1.373 (4)	C16—C17	1.375 (6)
O3—C3	1.428 (5)	C17—C18	1.387 (7)
O4—C10	1.253 (5)	C17—H17	0.9300
O4—Cd1^{iii}	2.351 (3)	C18—C19	1.363 (8)
O5—C10	1.257 (5)	C18—H18	0.9300
O5—Cd1^{iii}	2.370 (3)	C19—C20	1.338 (8)
N1—C11	1.329 (5)	C19—H19	0.9300
N1—C15	1.339 (5)	C20—H20	0.9300
N2—C16	1.345 (5)	O1w—H1w	0.8200
N2—C20	1.354 (6)	O1w—H2w	0.8200
C1—C2	1.507 (6)	O6—C21	1.244 (9)
C2—C3	1.511 (6)	O7—C21	1.263 (9)
C2—H2A	0.9700	O7—H7O	0.8200
C2—H2B	0.9700	O8—C25	1.375 (9)
C3—H3A	0.9700	O8—H8O	0.8200
C3—H3B	0.9700	C21—C22	1.495 (8)
C4—C9	1.366 (6)	C22—C23	1.3900
C4—C5	1.386 (6)	C22—C27	1.3900
C5—C6	1.385 (5)	C23—C24	1.3900
C5—H5	0.9300	C23—H23	0.9300
C6—C7	1.390 (6)	C24—C25	1.3900
C6—H6	0.9300	C24—H24	0.9300
C7—C8	1.379 (6)	C25—C26	1.3900
C7—C10	1.505 (5)	C26—C27	1.3900
C8—C9	1.388 (5)	C26—H26	0.9300
C8—H8	0.9300	C27—H27	0.9300
N2—Cd1—N1	71.09 (12)	C7—C8—H8	119.6
N2—Cd1—O2	132.62 (13)	C9—C8—H8	119.6
N1—Cd1—O2	99.56 (12)	C4—C9—C8	120.0 (4)
N2—Cd1—O4^{ii}	84.69 (13)	C4—C9—H9	120.0
N1—Cd1—O4^{ii}	114.25 (11)	C8—C9—H9	120.0
O2—Cd1—O4^{ii}	137.28 (11)	O4—C10—O5	122.2 (4)
N2—Cd1—O5^{ii}	98.40 (12)	O4—C10—C7	118.6 (4)
N1—Cd1—O5^{ii}	166.81 (11)	O5—C10—C7	119.2 (4)
O2—Cd1—O5^{ii}	93.44 (11)	N1—C11—C12	122.8 (5)
O4^{ii}—Cd1—O5^{ii}	55.46 (10)	N1—C11—H11	118.6
N2—Cd1—O2^{i}	150.29 (13)	C12—C11—H11	118.6
N1—Cd1—O2^{i}	88.75 (12)	C13—C12—C11	118.3 (5)
O2—Cd1—O2^{i}	70.79 (12)	C13—C12—H12	120.9
O4^{ii}—Cd1—O2^{i}	84.10 (11)	C11—C12—H12	120.9
O5^{ii}—Cd1—O2^{i}	97.67 (11)	C12—C13—C14	119.9 (5)
N2—Cd1—O1	80.37 (14)	C12—C13—H13	120.1
N1—Cd1—O1	83.43 (13)	C14—C13—H13	120.1
O2—Cd1—O1	52.26 (12)	C15—C14—C13	118.9 (5)

O4^{ii}—Cd1—O1	151.63 (12)	C15—C14—H14	120.5
O5^{ii}—Cd1—O1	103.05 (12)	C13—C14—H14	120.5
O2^{i}—Cd1—O1	119.78 (11)	N1—C15—C14	120.9 (4)
C1—O1—Cd1	89.9 (3)	N1—C15—C16	117.7 (4)
C1—O2—Cd1	97.7 (3)	C14—C15—C16	121.4 (4)
C1—O2—Cd1^{i}	144.3 (3)	N2—C16—C17	121.5 (4)
Cd1—O2—Cd1^{i}	109.21 (12)	N2—C16—C15	116.1 (4)
C4—O3—C3	119.1 (3)	C17—C16—C15	122.5 (4)
C10—O4—Cd1^{iii}	91.5 (2)	C16—C17—C18	119.6 (5)
C10—O5—Cd1^{iii}	90.5 (2)	C16—C17—H17	120.2
C11—N1—C15	119.2 (4)	C18—C17—H17	120.2
C11—N1—Cd1	123.7 (3)	C19—C18—C17	118.8 (5)
C15—N1—Cd1	116.9 (3)	C19—C18—H18	120.6
C16—N2—C20	116.9 (4)	C17—C18—H18	120.6
C16—N2—Cd1	118.1 (3)	C20—C19—C18	118.8 (5)
C20—N2—Cd1	124.9 (3)	C20—C19—H19	120.6
O1—C1—O2	119.9 (4)	C18—C19—H19	120.6
O1—C1—C2	119.1 (4)	C19—C20—N2	124.5 (5)
O2—C1—C2	121.0 (4)	C19—C20—H20	117.8
C1—C2—C3	112.5 (4)	N2—C20—H20	117.8
C1—C2—H2A	109.1	H1w—O1w—H2w	108.2
C3—C2—H2A	109.1	C21—O7—H7O	120.0
C1—C2—H2B	109.1	O6—C21—O7	120.8 (10)
C3—C2—H2B	109.1	O6—C21—C22	120.9 (9)
H2A—C2—H2B	107.8	O7—C21—C22	118.2 (10)
O3—C3—C2	105.8 (4)	C23—C22—C27	120.0
O3—C3—H3A	110.6	C23—C22—C21	119.5 (6)
C2—C3—H3A	110.6	C27—C22—C21	120.5 (6)
O3—C3—H3B	110.6	C22—C23—C24	120.0
C2—C3—H3B	110.6	C22—C23—H23	120.0
H3A—C3—H3B	108.7	C24—C23—H23	120.0
C9—C4—O3	115.8 (4)	C25—C24—C23	120.0
C9—C4—C5	120.5 (4)	C25—C24—H24	120.0
O3—C4—C5	123.7 (4)	C23—C24—H24	120.0
C6—C5—C4	119.1 (4)	O8—C25—C26	116.9 (6)
C6—C5—H5	120.4	O8—C25—C24	123.0 (6)
C4—C5—H5	120.4	C26—C25—C24	120.0
C5—C6—C7	121.0 (4)	C25—C26—C27	120.0
C5—C6—H6	119.5	C25—C26—H26	120.0
C7—C6—H6	119.5	C27—C26—H26	120.0
C8—C7—C6	118.6 (3)	C26—C27—C22	120.0
C8—C7—C10	121.3 (4)	C26—C27—H27	120.0
C6—C7—C10	120.0 (4)	C22—C27—H27	120.0
C7—C8—C9	120.8 (4)		
N2—Cd1—O1—C1	176.3 (3)	C4—C5—C6—C7	1.8 (7)
N1—Cd1—O1—C1	104.5 (3)	C5—C6—C7—C8	−0.7 (7)
O2—Cd1—O1—C1	−3.0 (2)	C5—C6—C7—C10	−177.8 (4)

O4^{ii}—Cd1—O1—C1	−124.5 (3)	C6—C7—C8—C9	0.3 (7)
O5^{ii}—Cd1—O1—C1	−87.2 (3)	C10—C7—C8—C9	177.3 (4)
O2^{i}—Cd1—O1—C1	19.7 (3)	O3—C4—C9—C8	−178.2 (4)
N2—Cd1—O2—C1	2.2 (3)	C5—C4—C9—C8	2.1 (7)
N1—Cd1—O2—C1	−70.9 (3)	C7—C8—C9—C4	−1.0 (7)
O4^{ii}—Cd1—O2—C1	146.4 (2)	Cd1^{iii}—O4—C10—O5	−6.1 (4)
O5^{ii}—Cd1—O2—C1	106.9 (3)	Cd1^{iii}—O4—C10—C7	173.3 (3)
O2^{i}—Cd1—O2—C1	−156.2 (3)	Cd1^{iii}—O5—C10—O4	6.0 (4)
O1—Cd1—O2—C1	3.0 (2)	Cd1^{iii}—O5—C10—C7	−173.3 (3)
N2—Cd1—O2—Cd1^{i}	158.33 (13)	C8—C7—C10—O4	−170.3 (4)
N1—Cd1—O2—Cd1^{i}	85.29 (14)	C6—C7—C10—O4	6.7 (6)
O4^{ii}—Cd1—O2—Cd1^{i}	−57.5 (2)	C8—C7—C10—O5	9.1 (6)
O5^{ii}—Cd1—O2—Cd1^{i}	−96.93 (14)	C6—C7—C10—O5	−173.9 (4)
O2^{i}—Cd1—O2—Cd1^{i}	0.0	C15—N1—C11—C12	0.2 (7)
O1—Cd1—O2—Cd1^{i}	159.2 (2)	Cd1—N1—C11—C12	175.3 (4)
N2—Cd1—N1—C11	−175.4 (4)	N1—C11—C12—C13	0.8 (9)
O2—Cd1—N1—C11	−43.5 (4)	C11—C12—C13—C14	0.2 (11)
O4^{ii}—Cd1—N1—C11	109.8 (4)	C12—C13—C14—C15	−2.2 (12)
O5^{ii}—Cd1—N1—C11	146.3 (5)	C11—N1—C15—C14	−2.3 (7)
O2^{i}—Cd1—N1—C11	26.8 (4)	Cd1—N1—C15—C14	−177.7 (4)
O1—Cd1—N1—C11	−93.4 (4)	C11—N1—C15—C16	177.0 (4)
N2—Cd1—N1—C15	−0.2 (3)	Cd1—N1—C15—C16	1.6 (5)
O2—Cd1—N1—C15	131.7 (3)	C13—C14—C15—N1	3.3 (9)
O4^{ii}—Cd1—N1—C15	−75.1 (3)	C13—C14—C15—C16	−176.0 (6)
O5^{ii}—Cd1—N1—C15	−38.5 (7)	C20—N2—C16—C17	0.8 (7)
O2^{i}—Cd1—N1—C15	−158.0 (3)	Cd1—N2—C16—C17	−177.2 (3)
O1—Cd1—N1—C15	81.8 (3)	C20—N2—C16—C15	−179.3 (5)
N1—Cd1—N2—C16	−1.4 (3)	Cd1—N2—C16—C15	2.6 (5)
O2—Cd1—N2—C16	−87.0 (3)	N1—C15—C16—N2	−2.9 (6)
O4^{ii}—Cd1—N2—C16	116.5 (3)	C14—C15—C16—N2	176.5 (5)
O5^{ii}—Cd1—N2—C16	170.4 (3)	N1—C15—C16—C17	177.0 (4)
O2^{i}—Cd1—N2—C16	48.3 (4)	C14—C15—C16—C17	−3.7 (7)
O1—Cd1—N2—C16	−87.7 (3)	N2—C16—C17—C18	−0.8 (7)
N1—Cd1—N2—C20	−179.2 (5)	C15—C16—C17—C18	179.4 (5)
O2—Cd1—N2—C20	95.2 (5)	C16—C17—C18—C19	−0.4 (8)
O4^{ii}—Cd1—N2—C20	−61.3 (5)	C17—C18—C19—C20	1.5 (10)
O5^{ii}—Cd1—N2—C20	−7.4 (5)	C18—C19—C20—N2	−1.5 (11)
O2^{i}—Cd1—N2—C20	−129.5 (5)	C16—N2—C20—C19	0.3 (9)
O1—Cd1—N2—C20	94.5 (5)	Cd1—N2—C20—C19	178.2 (5)
Cd1—O1—C1—O2	5.2 (4)	O6—C21—C22—C23	−12.1 (9)
Cd1—O1—C1—C2	−174.7 (3)	O7—C21—C22—C23	167.9 (9)
Cd1—O2—C1—O1	−5.6 (4)	O6—C21—C22—C27	169.2 (9)
Cd1^{i}—O2—C1—O1	−144.9 (4)	O7—C21—C22—C27	−10.8 (9)
Cd1—O2—C1—C2	174.3 (3)	C27—C22—C23—C24	0.0

Cd1^{i}—O2—C1—C2	35.1 (7)	C21—C22—C23—C24	−178.7 (10)
O1—C1—C2—C3	56.4 (6)	C22—C23—C24—C25	0.0
O2—C1—C2—C3	−123.5 (5)	C23—C24—C25—O8	175.3 (10)
C4—O3—C3—C2	−176.0 (4)	C23—C24—C25—C26	0.0
C1—C2—C3—O3	−172.8 (4)	O8—C25—C26—C27	−175.6 (10)
C3—O3—C4—C9	−173.5 (4)	C24—C25—C26—C27	0.0
C3—O3—C4—C5	6.2 (6)	C25—C26—C27—C22	0.0
C9—C4—C5—C6	−2.5 (7)	C23—C22—C27—C26	0.0
O3—C4—C5—C6	177.8 (4)	C21—C22—C27—C26	178.7 (10)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7o···O1w^{iv}	0.82	1.75	2.55 (1)	166
O8—H8o···O1	0.82	2.01	2.815 (8)	168
O1w—H1w···O1^{v}	0.82	1.98	2.797 (8)	171
O1w—H2w···O8	0.82	2.11	2.93 (1)	172

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

Fig. 1

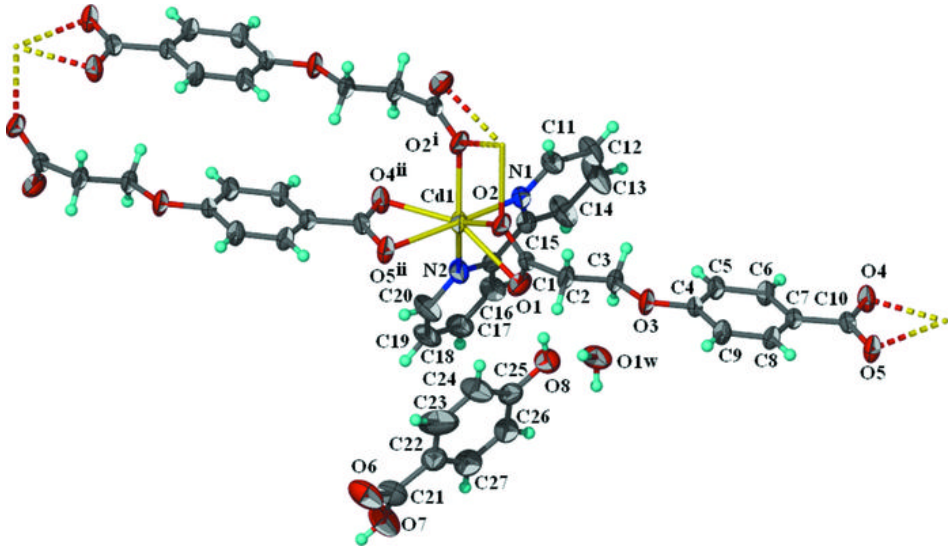

O2i
C11
C12
O4ii
N1
Cd1
O2
C13
C14
C15
O5ii
N2
C1
C3
C5
C6
O4
C20
C16
O1
C2
C4
C7
C10
O3
C19
C17
C18
O1w
C9
C8
O5
C24
C25
O8
C23
C26
C22
O6
C27
C21
O7

Fig. 2

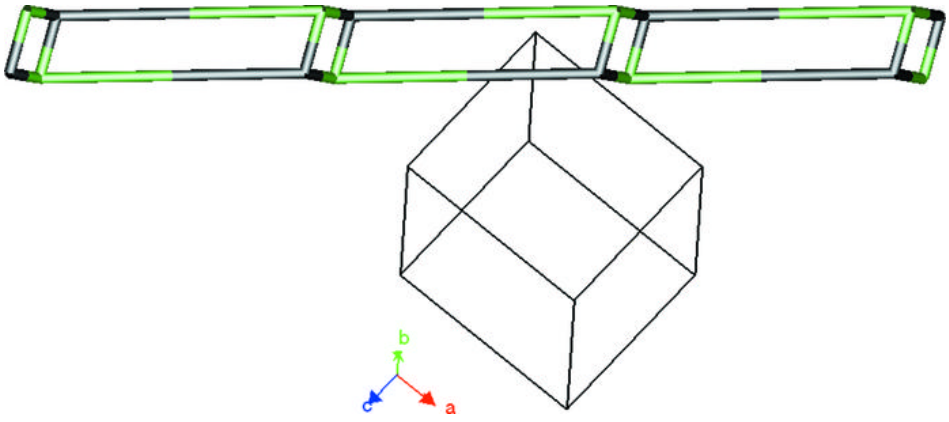


Fig. 3