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ISSN 2414-3146

Poly[bis[μ-4-(4-carboxyphenoxy)benzoato](μ-4,4′-oxydibenzoato)bis[μ-3-(pyridin-4-yl)-5-(pyridin-3-yl)-1*H*-1,2,4-triazole]dicadmium(II)]

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Received 16 June 2016
Accepted 6 July 2016

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

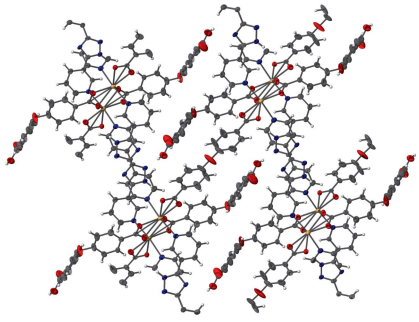
Keywords: crystal structure; coordination polymer; cadmium; oba; Hoba; 3,4′-bpt.

CCDC reference: 1490863

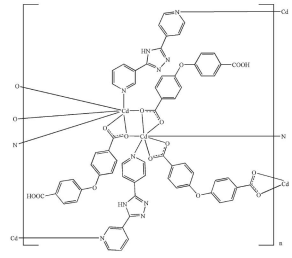
Structural data: full structural data are available from iucrdata.iucr.org

Three kinds of bridging ligands, 4,4′-oxydibenzoate, 4-(4-carboxyphenoxy)-benzoate and 3-(pyridin-4-yl)-5-(pyridin-3-yl)-1*H*-1,2,4-triazole, link the Cd^{II} cations to form the title polymeric complex, $[Cd_2(C_{14}H_8O_5)(C_{14}H_9O_5)_2(C_{12}H_9N_5)_2]_n$, in which each Cd^{II} cation is in a distorted N_2O_5 pentagonal–bipyramidal coordination geometry. The 4,4′-oxydibenzoate dianion exhibits point group symmetry 2, with the central O atom located on a twofold rotation axis. Classical N—H···O, O—H···N hydrogen bonds and weak C—H···O hydrogen bonds link the complex molecules into a three-dimensional supramolecular architecture. A solvent-accessible void of 53 (2) $Å^3$ is observed, but no solvent molecule could reasonably located there.

3D view



Chemical scheme



Structure description

Recently, coordination polymers (CPs) have been of interest in the field of crystal engineering, not only because of their potential applications as functional materials for fluorescence, magnetic materials, non-linear optics, ion exchange, catalysis and sorption (Yaghi *et al.*, 2003; Abrahams *et al.*, 1999; Yang *et al.*, 2008), but also because of their intriguing aesthetic structures and topologies (Dong *et al.*, 2007; Huang *et al.*, 2013). Coordination polymeric frameworks can be rationally designed by careful control of many factors such as the solvent system, temperature, pH value, the metal-to-ligand ratio, geometric requirements of metal ions and secondary building-block ligands.

The V-shaped organic aromatic multicarboxylate species, H_2oba (4,4′-oxydibenzoic acid), have been extensively employed as building blocks to construct coordination polymeric frameworks (Huang *et al.*, 2010; Lan *et al.*, 2008; Yao *et al.*, 2013) because they show various coordination modes with metal ions, which give rise to a great variety of

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O6^{ii}	0.86	1.85	2.695 (5)	169
O4—H4···N2^{iii}	0.82	2.06	2.848 (5)	162
C3—H3···O6^{ii}	0.93	2.40	3.285 (5)	158
C25—H25···O3^{iv}	0.93	2.37	3.238 (8)	154

Symmetry codes: (ii) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $x, y-1, z$.

multi-dimensional structures and fascinating topologies. On the other hand, a mixed-ligand strategy is presently a good choice for the construction of coordination polymers. Careful selection of the properties of the secondary ligands, such as shape, functionality, flexibility, angle and symmetry, is therefore key for the rational design of structures and specific chemical and physical properties. In the present case, we have prepared the title compound, $[Cd_2(oba)(Hoba)_2(3,4'\text{-bpt})_2]_n$, using H_2oba and 3,4′-bpt.

The asymmetric unit comprises of one independent Cd^{II} cation, one 3,4′-bpt ligand and one $Hoba^-$ ligand and a half oba^{2-} ligand. Each Cd^{II} cation is coordinated by two nitrogen atoms, occupying the axial positions, from two different 3,4′-bpt ligands and five oxygen atoms, occupying the equatorial positions, from three different oba^{2-} ligands (Fig. 1). This binding mode forms a distorted pentagonal–bipyramid coordination geometry around each metal ion with Cd—N(py) distances of 2.310 (3) and 2.366 (3) Å and Cd—O (carboxylate) distance of 2.274 (3)-2.598 (3) Å, similar to that observed in previously reported Cd^{II} complexes. The oba^{2-} and 3,4′-bpt ligands connect the Cd^{II} cations, forming a three-dimensional framework. The $Hoba^-$ ligands are bound only through their carboxylate group to the cation, whereas the carboxyl group is non-coordinating (Fig. 2). Classical N—H···O and O—H···N hydrogen bonds and weak C—H···O interactions (Table 1) link the complex molecules into a three-dimensional supramolecular architecture.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cd_2(C_{14}H_8O_5)(C_{14}H_9O_5)_2(C_{12}H_9N_5)_2]$
M_r	1441.91
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	298
a, b, c (Å)	27.471 (3), 7.4230 (6), 31.425 (3)
β (°)	108.428 (3)
V (Å^3)	6079.5 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.78
Crystal size (mm)	0.20 × 0.14 × 0.11
Data collection	
Diffractometer	Bruker SMART 1000 CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.86, 0.92
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14594, 5323, 3773
R_{int}	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.107, 1.04
No. of reflections	5323
No. of parameters	421
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.65, −0.68

Computer programs: *SMART* and *SAINT* (Bruker, 2007) and *SHELXTL* (Sheldrick, 2008).

Synthesis and crystallization

Materials and physical measurements

All reagents and solvents were purchased from commercial sources and used as received. Elemental analysis for carbon, hydrogen and nitrogen were carried out on a Perkin–Elmer elemental analyzer model 240. Infrared spectra were taken on a Bruker Tensor 27 Fourier transform IR spectroscope in the region 4000–400 cm^{-1}, using KBr pellets.

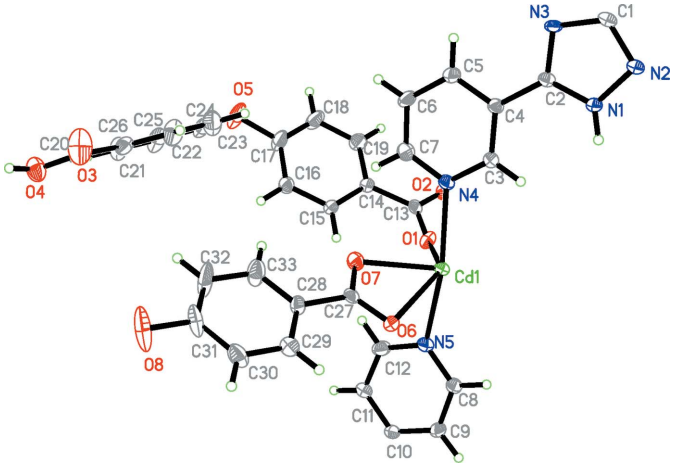


Figure 1
The asymmetric unit of the title complex, with 50% probability displacement ellipsoids.

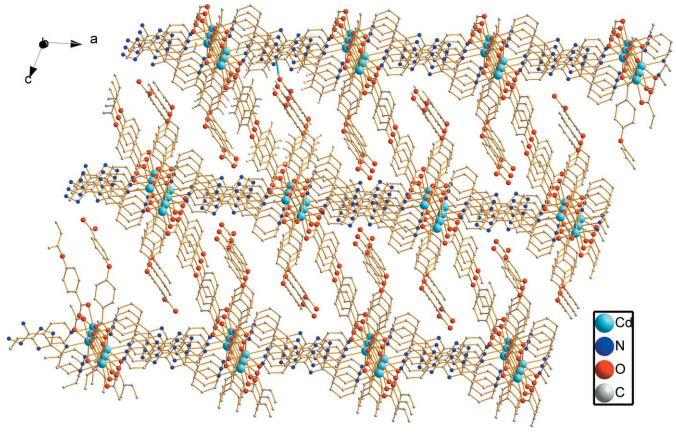


Figure 2
The polymeric structure of the title complex.

Synthesis of $[Cd(Hoba)(oba)_{0.5}(3,4'\text{-bpt})_2]_n$

A mixture of $Cd(OAc)_2{\cdot}H_2O$ (8 mg, 0.03 mmol), H2oba (7.7 mg, 0.06 mmol), and 3,4′-bpt (6.6 mg, 0.03 mmol) was dissolved in distilled water (7 ml), and then sealed in a 23-ml Teflon-lined stainless steel autoclave and heated at 433 K for 5 d under autogenous pressure. Then the mixture was cooled to room temperature at a rate of 5 K h^{-1}, and colourless crystals were obtained in a 42% yield based on Cd^{II}. FT–IR (KBr pellet, cm^{-1}): 3121 (*w*), 1608 (*s*), 1549 (*s*), 1494 (*m*), 1476 (*m*), 1412 (*s*), 1356 (*s*), 1298 (*w*), 1232 (*s*), 1155 (*m*), 873 (*m*), 844 (*w*), 771 (*m*), 694 (*w*).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We thank the Ningxia Natural Science Foundation of China (grant No. NZ14232).

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full crystallographic data

IUCrData (2016). **1**, x161092 [https://doi.org/10.1107/S2414314616010920]

Poly[bis[μ-4-(4-carboxyphenoxy)benzoato](μ-4,4′-oxydibenzoato)bis[μ-3-(pyridin-4-yl)-5-(pyridin-3-yl)-1*H*-1,2,4-triazole]dicadmium(II)]

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Crystal data

$[Cd_2(C_{14}H_8O_5)(C_{14}H_9O_5)_2(C_{12}H_9N_5)_2]$
M_r = 1441.91
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 27.471 (3) Å
b = 7.4230 (6) Å
c = 31.425 (3) Å
β = 108.428 (3)°
V = 6079.5 (9) Å^3
Z = 4
F(000) = 2904
D_x = 1.575 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 3641 reflections
θ = 2.4–24.3°
μ = 0.78 mm^{-1}
T = 298 K
Block, colorless
0.20 × 0.14 × 0.11 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.86, T_{max} = 0.92
14594 measured reflections
5323 independent reflections
3773 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −31→32
k = −8→8
l = −37→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.107
S = 1.04
5323 reflections
421 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.9862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.289097 (11)	0.46259 (5)	0.030672 (11)	0.02920 (13)
N1	0.07438 (13)	0.7187 (5)	−0.01858 (12)	0.0294 (9)
H1	0.0956	0.7252	−0.0336	0.035*
N2	0.02470 (13)	0.7750 (5)	−0.03350 (12)	0.0297 (9)
N3	0.04482 (12)	0.6626 (5)	0.03668 (11)	0.0267 (9)
N4	0.22153 (13)	0.4928 (5)	0.05906 (12)	0.0293 (10)
N5	0.36097 (13)	0.3577 (6)	0.01178 (12)	0.0329 (10)
O1	0.28217 (12)	0.1455 (5)	0.04089 (10)	0.0358 (8)
O2	0.23531 (11)	−0.0955 (5)	0.03804 (10)	0.0361 (8)
O3	0.42338 (18)	0.7322 (6)	0.35543 (14)	0.0800 (14)
O4	0.47900 (14)	0.5180 (5)	0.38766 (13)	0.0539 (10)
H4	0.4907	0.5968	0.4064	0.081*
O5	0.32055 (18)	0.0274 (6)	0.24857 (12)	0.0777 (15)
O6	0.35603 (11)	0.7166 (5)	0.06091 (10)	0.0342 (8)
O7	0.33973 (12)	0.5070 (5)	0.10412 (10)	0.0381 (9)
O8	0.5000	0.9873 (7)	0.2500	0.090 (2)
C1	0.00927 (15)	0.7377 (6)	0.00170 (15)	0.0281 (11)
C2	0.08526 (15)	0.6516 (6)	0.02293 (14)	0.0251 (10)
C3	0.17640 (15)	0.5611 (6)	0.03435 (14)	0.0300 (11)
H3	0.1727	0.5992	0.0053	0.036*
C4	0.13503 (15)	0.5775 (6)	0.05022 (14)	0.0271 (11)
C5	0.14072 (18)	0.5158 (7)	0.09313 (15)	0.0409 (14)
H5	0.1134	0.5217	0.1046	0.049*
C6	0.18669 (18)	0.4467 (8)	0.11829 (16)	0.0470 (15)
H6	0.1912	0.4054	0.1472	0.056*
C7	0.22616 (18)	0.4386 (7)	0.10063 (16)	0.0382 (13)
H7	0.2576	0.3933	0.1184	0.046*
C8	0.37231 (16)	0.3992 (7)	−0.02542 (15)	0.0333 (12)
H8	0.3474	0.4559	−0.0488	0.040*
C9	0.41953 (16)	0.3614 (7)	−0.03072 (15)	0.0359 (12)
H9	0.4259	0.3930	−0.0571	0.043*
C10	0.45670 (16)	0.2770 (6)	0.00319 (14)	0.0274 (11)
C11	0.44514 (17)	0.2305 (7)	0.04141 (16)	0.0358 (12)
H11	0.4692	0.1722	0.0650	0.043*
C12	0.39741 (18)	0.2718 (7)	0.04391 (17)	0.0400 (13)

H12	0.3899	0.2378	0.0696	0.048*
C13	0.26637 (16)	0.0196 (7)	0.06003 (15)	0.0281 (11)
C14	0.28350 (16)	0.0110 (6)	0.11004 (14)	0.0293 (11)
C15	0.32486 (16)	0.1127 (7)	0.13509 (14)	0.0302 (11)
H15	0.3438	0.1778	0.1206	0.036*
C16	0.33845 (17)	0.1191 (7)	0.18129 (15)	0.0364 (12)
H16	0.3668	0.1859	0.1978	0.044*
C17	0.3099 (2)	0.0266 (8)	0.20264 (16)	0.0498 (15)
C18	0.2697 (2)	−0.0800 (9)	0.17870 (17)	0.0587 (17)
H18	0.2514	−0.1467	0.1936	0.070*
C19	0.25647 (19)	−0.0883 (8)	0.13231 (16)	0.0464 (14)
H19	0.2293	−0.1608	0.1161	0.056*
C20	0.4371 (2)	0.5775 (9)	0.35748 (18)	0.0476 (15)
C21	0.40777 (19)	0.4321 (8)	0.32755 (15)	0.0398 (13)
C22	0.3641 (2)	0.4764 (9)	0.29242 (19)	0.0603 (17)
H22	0.3544	0.5964	0.2870	0.072*
C23	0.3352 (2)	0.3426 (11)	0.2656 (2)	0.0687 (19)
H23	0.3056	0.3721	0.2424	0.082*
C24	0.3501 (2)	0.1671 (9)	0.27310 (17)	0.0544 (17)
C25	0.3937 (2)	0.1211 (9)	0.30754 (18)	0.0581 (16)
H25	0.4041	0.0016	0.3126	0.070*
C26	0.4211 (2)	0.2561 (8)	0.33417 (17)	0.0524 (15)
H26	0.4502	0.2258	0.3578	0.063*
C27	0.36363 (15)	0.6449 (7)	0.09910 (15)	0.0288 (11)
C28	0.40157 (17)	0.7291 (7)	0.13951 (15)	0.0318 (11)
C29	0.42965 (17)	0.8779 (8)	0.13527 (17)	0.0414 (13)
H29	0.4256	0.9248	0.1069	0.050*
C30	0.46327 (19)	0.9576 (8)	0.17205 (18)	0.0502 (14)
H30	0.4826	1.0563	0.1688	0.060*
C31	0.4681 (2)	0.8909 (9)	0.21363 (18)	0.0572 (17)
C32	0.4408 (3)	0.7453 (9)	0.21871 (19)	0.078 (2)
H32	0.4447	0.7002	0.2472	0.094*
C33	0.4070 (2)	0.6642 (8)	0.18155 (18)	0.0624 (18)
H33	0.3879	0.5652	0.1851	0.075*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01983 (18)	0.0412 (2)	0.0273 (2)	−0.00041 (17)	0.00838 (13)	−0.00007 (17)
N1	0.0235 (19)	0.040 (3)	0.028 (2)	0.0058 (18)	0.0120 (17)	0.0039 (18)
N2	0.0222 (19)	0.038 (3)	0.032 (2)	0.0040 (18)	0.0123 (17)	0.0012 (18)
N3	0.0226 (19)	0.032 (3)	0.031 (2)	0.0021 (17)	0.0163 (17)	0.0016 (18)
N4	0.0228 (19)	0.035 (3)	0.030 (2)	0.0053 (17)	0.0094 (16)	−0.0018 (17)
N5	0.026 (2)	0.041 (3)	0.034 (2)	0.0002 (19)	0.0129 (18)	−0.0012 (19)
O1	0.046 (2)	0.036 (2)	0.0262 (18)	0.0050 (17)	0.0135 (15)	0.0043 (15)
O2	0.0327 (17)	0.047 (2)	0.0252 (17)	−0.0099 (17)	0.0040 (14)	−0.0013 (16)
O3	0.102 (4)	0.046 (3)	0.071 (3)	0.013 (3)	−0.003 (3)	−0.005 (2)
O4	0.048 (2)	0.051 (3)	0.055 (3)	0.000 (2)	0.0047 (19)	−0.0138 (19)

O5	0.114 (4)	0.090 (4)	0.027 (2)	−0.057 (3)	0.018 (2)	−0.007 (2)
O6	0.0272 (16)	0.051 (2)	0.0250 (18)	0.0008 (16)	0.0097 (14)	0.0039 (16)
O7	0.0352 (18)	0.042 (3)	0.0345 (19)	−0.0109 (17)	0.0066 (15)	−0.0044 (16)
O8	0.103 (5)	0.037 (4)	0.072 (4)	0.000	−0.055 (4)	0.000
C1	0.021 (2)	0.027 (3)	0.039 (3)	0.001 (2)	0.013 (2)	−0.003 (2)
C2	0.024 (2)	0.021 (3)	0.033 (3)	0.001 (2)	0.012 (2)	0.002 (2)
C3	0.025 (2)	0.037 (3)	0.027 (2)	0.002 (2)	0.008 (2)	0.002 (2)
C4	0.025 (2)	0.028 (3)	0.030 (3)	0.005 (2)	0.0101 (19)	0.004 (2)
C5	0.033 (3)	0.060 (4)	0.033 (3)	0.013 (3)	0.016 (2)	0.006 (3)
C6	0.044 (3)	0.070 (4)	0.032 (3)	0.019 (3)	0.020 (2)	0.022 (3)
C7	0.034 (3)	0.040 (4)	0.040 (3)	0.014 (2)	0.011 (2)	0.009 (2)
C8	0.026 (2)	0.042 (3)	0.032 (3)	0.005 (2)	0.010 (2)	0.001 (2)
C9	0.031 (3)	0.050 (4)	0.030 (3)	0.006 (2)	0.015 (2)	0.005 (2)
C10	0.026 (2)	0.028 (3)	0.030 (3)	−0.003 (2)	0.012 (2)	−0.004 (2)
C11	0.026 (2)	0.044 (4)	0.038 (3)	0.000 (2)	0.011 (2)	0.001 (2)
C12	0.038 (3)	0.047 (4)	0.041 (3)	0.007 (3)	0.021 (2)	0.008 (3)
C13	0.021 (2)	0.034 (3)	0.028 (3)	0.009 (2)	0.007 (2)	0.001 (2)
C14	0.027 (2)	0.033 (3)	0.028 (2)	0.001 (2)	0.009 (2)	0.001 (2)
C15	0.031 (2)	0.036 (3)	0.025 (2)	0.001 (2)	0.011 (2)	0.004 (2)
C16	0.036 (3)	0.039 (3)	0.032 (3)	−0.010 (2)	0.007 (2)	−0.002 (2)
C17	0.067 (4)	0.055 (4)	0.025 (3)	−0.019 (3)	0.012 (3)	0.000 (3)
C18	0.072 (4)	0.075 (5)	0.033 (3)	−0.032 (4)	0.022 (3)	−0.003 (3)
C19	0.047 (3)	0.053 (4)	0.040 (3)	−0.025 (3)	0.016 (3)	−0.006 (3)
C20	0.054 (4)	0.049 (4)	0.043 (3)	−0.003 (3)	0.020 (3)	−0.003 (3)
C21	0.046 (3)	0.045 (4)	0.031 (3)	0.001 (3)	0.016 (2)	−0.003 (3)
C22	0.070 (4)	0.059 (4)	0.045 (3)	0.013 (3)	0.008 (3)	−0.004 (3)
C23	0.058 (4)	0.090 (6)	0.049 (4)	0.002 (4)	0.003 (3)	−0.010 (4)
C24	0.075 (4)	0.063 (5)	0.028 (3)	−0.025 (4)	0.020 (3)	−0.007 (3)
C25	0.086 (4)	0.050 (4)	0.034 (3)	−0.010 (4)	0.012 (3)	−0.001 (3)
C26	0.058 (4)	0.052 (4)	0.039 (3)	−0.001 (3)	0.004 (3)	0.001 (3)
C27	0.017 (2)	0.042 (3)	0.028 (3)	0.005 (2)	0.0072 (19)	−0.006 (2)
C28	0.031 (2)	0.032 (3)	0.028 (3)	0.003 (2)	0.002 (2)	0.004 (2)
C29	0.035 (3)	0.047 (4)	0.041 (3)	−0.002 (3)	0.010 (2)	0.001 (3)
C30	0.037 (3)	0.047 (4)	0.058 (4)	−0.013 (3)	0.002 (3)	0.000 (3)
C31	0.053 (3)	0.043 (4)	0.048 (4)	0.001 (3)	−0.024 (3)	−0.008 (3)
C32	0.115 (5)	0.062 (5)	0.028 (3)	−0.024 (4)	−0.019 (3)	0.014 (3)
C33	0.077 (4)	0.056 (4)	0.039 (3)	−0.030 (4)	−0.003 (3)	0.010 (3)

Geometric parameters (Å, º)

Cd1—O1	2.391 (4)	C8—H8	0.9300
Cd1—O1^{i}	2.598 (3)	C9—C10	1.372 (6)
Cd1—O2^{i}	2.274 (3)	C9—H9	0.9300
Cd1—O6	2.595 (3)	C10—C11	1.380 (6)
Cd1—O7	2.311 (3)	C10—C1^{iv}	1.488 (5)
Cd1—N4	2.310 (3)	C11—C12	1.373 (6)
Cd1—N5	2.366 (3)	C11—H11	0.9300
N1—C2	1.339 (5)	C12—H12	0.9300

N1—N2	1.361 (4)	C13—C14	1.493 (6)
N1—H1	0.8600	C14—C19	1.383 (6)
N2—C1	1.333 (5)	C14—C15	1.384 (6)
N3—C2	1.316 (5)	C15—C16	1.381 (6)
N3—C1	1.339 (5)	C15—H15	0.9300
N4—C7	1.334 (6)	C16—C17	1.368 (6)
N4—C3	1.337 (5)	C16—H16	0.9300
N5—C12	1.338 (6)	C17—C18	1.373 (7)
N5—C8	1.337 (5)	C18—C19	1.388 (7)
O1—C13	1.260 (5)	C18—H18	0.9300
O1—Cd1^{i}	2.598 (3)	C19—H19	0.9300
O2—C13	1.250 (5)	C20—C21	1.490 (8)
O2—Cd1^{i}	2.274 (3)	C21—C26	1.355 (7)
O3—C20	1.205 (7)	C21—C22	1.388 (7)
O4—C20	1.315 (6)	C22—C23	1.381 (8)
O4—H4	0.8200	C22—H22	0.9300
O5—C17	1.379 (6)	C23—C24	1.364 (9)
O5—C24	1.391 (7)	C23—H23	0.9300
O6—C27	1.268 (5)	C24—C25	1.378 (8)
O7—C27	1.253 (5)	C25—C26	1.369 (8)
O8—C31	1.397 (6)	C25—H25	0.9300
O8—C31^{ii}	1.397 (6)	C26—H26	0.9300
C1—C10^{iii}	1.488 (5)	C27—C28	1.501 (6)
C2—C4	1.472 (6)	C28—C33	1.369 (7)
C3—C4	1.383 (5)	C28—C29	1.378 (7)
C3—H3	0.9300	C29—C30	1.365 (7)
C4—C5	1.385 (6)	C29—H29	0.9300
C5—C6	1.361 (6)	C30—C31	1.364 (8)
C5—H5	0.9300	C30—H30	0.9300
C6—C7	1.367 (6)	C31—C32	1.355 (8)
C6—H6	0.9300	C32—C33	1.379 (7)
C7—H7	0.9300	C32—H32	0.9300
C8—C9	1.388 (6)	C33—H33	0.9300

O2^{i}—Cd1—N4	107.04 (12)	C11—C10—C1^{iv}	118.1 (4)
O2^{i}—Cd1—O7	142.22 (12)	C12—C11—C10	118.7 (5)
N4—Cd1—O7	84.49 (12)	C12—C11—H11	120.6
O2^{i}—Cd1—N5	85.60 (12)	C10—C11—H11	120.6
N4—Cd1—N5	164.75 (14)	N5—C12—C11	124.3 (4)
O7—Cd1—N5	90.63 (12)	N5—C12—H12	117.8
O2^{i}—Cd1—O1	122.85 (11)	C11—C12—H12	117.8
N4—Cd1—O1	86.32 (12)	O2—C13—O1	121.4 (4)
O7—Cd1—O1	93.13 (11)	O2—C13—C14	119.1 (4)
N5—Cd1—O1	79.51 (12)	O1—C13—C14	119.5 (4)
O2^{i}—Cd1—O6	89.69 (11)	C19—C14—C15	118.6 (4)
N4—Cd1—O6	110.55 (11)	C19—C14—C13	121.0 (4)
O7—Cd1—O6	52.96 (10)	C15—C14—C13	120.3 (4)
N5—Cd1—O6	77.29 (12)	C16—C15—C14	121.2 (4)

O1—Cd1—O6	138.01 (10)	C16—C15—H15	119.4
O2^{i}—Cd1—O1^{i}	52.89 (11)	C14—C15—H15	119.4
N4—Cd1—O1^{i}	83.49 (11)	C17—C16—C15	119.5 (4)
O7—Cd1—O1^{i}	163.63 (11)	C17—C16—H16	120.3
N5—Cd1—O1^{i}	98.13 (11)	C15—C16—H16	120.3
O1—Cd1—O1^{i}	75.05 (11)	C16—C17—C18	120.4 (5)
O6—Cd1—O1^{i}	142.57 (10)	C16—C17—O5	123.1 (5)
C2—N1—N2	109.9 (3)	C18—C17—O5	116.4 (5)
C2—N1—H1	125.0	C17—C18—C19	120.0 (5)
N2—N1—H1	125.0	C17—C18—H18	120.0
C1—N2—N1	101.4 (3)	C19—C18—H18	120.0
C2—N3—C1	103.2 (3)	C14—C19—C18	120.2 (5)
C7—N4—C3	117.8 (4)	C14—C19—H19	119.9
C7—N4—Cd1	120.6 (3)	C18—C19—H19	119.9
C3—N4—Cd1	121.5 (3)	O3—C20—O4	123.1 (5)
C12—N5—C8	116.4 (4)	O3—C20—C21	124.0 (6)
C12—N5—Cd1	116.9 (3)	O4—C20—C21	112.8 (5)
C8—N5—Cd1	125.9 (3)	C26—C21—C22	118.3 (5)
C13—O1—Cd1	148.0 (3)	C26—C21—C20	122.4 (5)
C13—O1—Cd1^{i}	84.6 (3)	C22—C21—C20	119.3 (6)
Cd1—O1—Cd1^{i}	104.95 (11)	C23—C22—C21	120.1 (6)
C13—O2—Cd1^{i}	100.0 (3)	C23—C22—H22	120.0
C20—O4—H4	109.5	C21—C22—H22	120.0
C17—O5—C24	118.5 (4)	C24—C23—C22	119.8 (6)
C27—O6—Cd1	85.8 (3)	C24—C23—H23	120.1
C27—O7—Cd1	99.5 (3)	C22—C23—H23	120.1
C31—O8—C31^{ii}	118.4 (6)	C23—C24—C25	120.8 (6)
N2—C1—N3	115.3 (4)	C23—C24—O5	121.7 (6)
N2—C1—C10^{iii}	123.5 (4)	C25—C24—O5	117.4 (6)
N3—C1—C10^{iii}	121.2 (4)	C26—C25—C24	118.2 (6)
N3—C2—N1	110.2 (4)	C26—C25—H25	120.9
N3—C2—C4	123.9 (4)	C24—C25—H25	120.9
N1—C2—C4	125.9 (4)	C21—C26—C25	122.8 (5)
N4—C3—C4	122.7 (4)	C21—C26—H26	118.6
N4—C3—H3	118.6	C25—C26—H26	118.6
C4—C3—H3	118.6	O7—C27—O6	121.7 (4)
C3—C4—C5	118.0 (4)	O7—C27—C28	119.0 (4)
C3—C4—C2	122.7 (4)	O6—C27—C28	119.2 (5)
C5—C4—C2	119.3 (4)	C33—C28—C29	118.8 (5)
C6—C5—C4	119.2 (4)	C33—C28—C27	120.3 (5)
C6—C5—H5	120.4	C29—C28—C27	120.8 (4)
C4—C5—H5	120.4	C30—C29—C28	121.0 (5)
C5—C6—C7	119.4 (4)	C30—C29—H29	119.5
C5—C6—H6	120.3	C28—C29—H29	119.5
C7—C6—H6	120.3	C31—C30—C29	119.3 (5)
N4—C7—C6	122.8 (4)	C31—C30—H30	120.4
N4—C7—H7	118.6	C29—C30—H30	120.4
C6—C7—H7	118.6	C32—C31—C30	120.8 (5)

N5—C8—C9	122.9 (4)	C32—C31—O8	122.7 (5)
N5—C8—H8	118.5	C30—C31—O8	116.4 (6)
C9—C8—H8	118.5	C31—C32—C33	119.9 (5)
C10—C9—C8	119.6 (4)	C31—C32—H32	120.0
C10—C9—H9	120.2	C33—C32—H32	120.0
C8—C9—H9	120.2	C28—C33—C32	120.1 (6)
C9—C10—C11	118.1 (4)	C28—C33—H33	119.9
C9—C10—C1^{iv}	123.8 (4)	C32—C33—H33	119.9
C2—N1—N2—C1	0.6 (5)	C5—C6—C7—N4	−1.3 (9)
O2^{i}—Cd1—N4—C7	−175.1 (3)	C12—N5—C8—C9	−1.8 (7)
O7—Cd1—N4—C7	−31.9 (4)	Cd1—N5—C8—C9	167.5 (4)
N5—Cd1—N4—C7	39.9 (7)	N5—C8—C9—C10	0.3 (8)
O1—Cd1—N4—C7	61.6 (4)	C8—C9—C10—C11	0.9 (7)
O6—Cd1—N4—C7	−78.9 (4)	C8—C9—C10—C1^{iv}	−177.2 (4)
O1^{i}—Cd1—N4—C7	136.9 (4)	C9—C10—C11—C12	−0.5 (7)
O2^{i}—Cd1—N4—C3	6.3 (4)	C1^{iv}—C10—C11—C12	177.7 (5)
O7—Cd1—N4—C3	149.5 (4)	C8—N5—C12—C11	2.2 (8)
N5—Cd1—N4—C3	−138.7 (5)	Cd1—N5—C12—C11	−168.1 (4)
O1—Cd1—N4—C3	−117.0 (4)	C10—C11—C12—N5	−1.1 (8)
O6—Cd1—N4—C3	102.5 (3)	Cd1^{i}—O2—C13—O1	−12.0 (5)
O1^{i}—Cd1—N4—C3	−41.7 (3)	Cd1^{i}—O2—C13—C14	165.8 (3)
O2^{i}—Cd1—N5—C12	173.7 (4)	Cd1—O1—C13—O2	120.0 (5)
N4—Cd1—N5—C12	−39.6 (7)	Cd1^{i}—O1—C13—O2	10.3 (4)
O7—Cd1—N5—C12	31.4 (4)	Cd1—O1—C13—C14	−57.7 (7)
O1—Cd1—N5—C12	−61.7 (4)	Cd1^{i}—O1—C13—C14	−167.4 (4)
O6—Cd1—N5—C12	83.1 (4)	O2—C13—C14—C19	−17.1 (7)
O1^{i}—Cd1—N5—C12	−134.7 (4)	O1—C13—C14—C19	160.7 (5)
O2^{i}—Cd1—N5—C8	4.4 (4)	O2—C13—C14—C15	167.4 (4)
N4—Cd1—N5—C8	151.1 (5)	O1—C13—C14—C15	−14.9 (6)
O7—Cd1—N5—C8	−137.9 (4)	C19—C14—C15—C16	−1.5 (7)
O1—Cd1—N5—C8	129.0 (4)	C13—C14—C15—C16	174.1 (4)
O6—Cd1—N5—C8	−86.2 (4)	C14—C15—C16—C17	−1.4 (8)
O1^{i}—Cd1—N5—C8	56.0 (4)	C15—C16—C17—C18	3.6 (9)
O2^{i}—Cd1—O1—C13	−127.7 (5)	C15—C16—C17—O5	−179.4 (5)
N4—Cd1—O1—C13	−19.8 (5)	C24—O5—C17—C16	20.8 (9)
O7—Cd1—O1—C13	64.5 (5)	C24—O5—C17—C18	−162.1 (6)
N5—Cd1—O1—C13	154.5 (5)	C16—C17—C18—C19	−2.8 (10)
O6—Cd1—O1—C13	97.2 (5)	O5—C17—C18—C19	180.0 (5)
O1^{i}—Cd1—O1—C13	−104.0 (6)	C15—C14—C19—C18	2.3 (8)
O2^{i}—Cd1—O1—Cd1^{i}	−23.70 (16)	C13—C14—C19—C18	−173.3 (5)
N4—Cd1—O1—Cd1^{i}	84.24 (12)	C17—C18—C19—C14	−0.2 (9)
O7—Cd1—O1—Cd1^{i}	168.50 (11)	O3—C20—C21—C26	−172.0 (6)
N5—Cd1—O1—Cd1^{i}	−101.44 (13)	O4—C20—C21—C26	5.8 (7)
O6—Cd1—O1—Cd1^{i}	−158.75 (10)	O3—C20—C21—C22	5.8 (8)
O1^{i}—Cd1—O1—Cd1^{i}	0.0	O4—C20—C21—C22	−176.4 (5)
O2^{i}—Cd1—O6—C27	173.6 (2)	C26—C21—C22—C23	0.8 (8)
N4—Cd1—O6—C27	65.5 (3)	C20—C21—C22—C23	−177.1 (5)

O7—Cd1—O6—C27	−0.2 (2)	C21—C22—C23—C24	−1.3 (9)
N5—Cd1—O6—C27	−100.8 (3)	C22—C23—C24—C25	0.6 (9)
O1—Cd1—O6—C27	−42.8 (3)	C22—C23—C24—O5	176.2 (5)
O1^{i}—Cd1—O6—C27	172.4 (2)	C17—O5—C24—C23	59.4 (8)
O2^{i}—Cd1—O7—C27	−9.9 (4)	C17—O5—C24—C25	−124.9 (6)
N4—Cd1—O7—C27	−120.8 (3)	C23—C24—C25—C26	0.6 (9)
N5—Cd1—O7—C27	73.7 (3)	O5—C24—C25—C26	−175.2 (5)
O1—Cd1—O7—C27	153.3 (3)	C22—C21—C26—C25	0.4 (9)
O6—Cd1—O7—C27	0.2 (2)	C20—C21—C26—C25	178.3 (5)
O1^{i}—Cd1—O7—C27	−163.7 (3)	C24—C25—C26—C21	−1.1 (9)
N1—N2—C1—N3	−0.4 (5)	Cd1—O7—C27—O6	−0.4 (5)
N1—N2—C1—C10^{iii}	178.9 (4)	Cd1—O7—C27—C28	178.6 (3)
C2—N3—C1—N2	0.0 (5)	Cd1—O6—C27—O7	0.4 (4)
C2—N3—C1—C10^{iii}	−179.3 (4)	Cd1—O6—C27—C28	−178.6 (4)
C1—N3—C2—N1	0.4 (5)	O7—C27—C28—C33	−5.0 (7)
C1—N3—C2—C4	179.7 (4)	O6—C27—C28—C33	174.0 (5)
N2—N1—C2—N3	−0.7 (5)	O7—C27—C28—C29	178.2 (4)
N2—N1—C2—C4	180.0 (4)	O6—C27—C28—C29	−2.8 (7)
C7—N4—C3—C4	0.1 (7)	C33—C28—C29—C30	1.5 (8)
Cd1—N4—C3—C4	178.7 (3)	C27—C28—C29—C30	178.3 (4)
N4—C3—C4—C5	−1.7 (7)	C28—C29—C30—C31	−1.5 (8)
N4—C3—C4—C2	−179.6 (4)	C29—C30—C31—C32	1.1 (9)
N3—C2—C4—C3	177.5 (4)	C29—C30—C31—O8	−175.0 (5)
N1—C2—C4—C3	−3.3 (7)	C31^{ii}—O8—C31—C32	43.9 (5)
N3—C2—C4—C5	−0.4 (7)	C31^{ii}—O8—C31—C30	−140.1 (6)
N1—C2—C4—C5	178.8 (5)	C30—C31—C32—C33	−0.8 (11)
C3—C4—C5—C6	1.7 (8)	O8—C31—C32—C33	175.0 (6)
C2—C4—C5—C6	179.8 (5)	C29—C28—C33—C32	−1.2 (9)
C4—C5—C6—C7	−0.4 (8)	C27—C28—C33—C32	−178.0 (5)
C3—N4—C7—C6	1.4 (7)	C31—C32—C33—C28	0.8 (11)
Cd1—N4—C7—C6	−177.3 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O6^{v}	0.86	1.85	2.695 (5)	169
O4—H4···N2^{vi}	0.82	2.06	2.848 (5)	162
C3—H3···O6^{v}	0.93	2.40	3.285 (5)	158
C25—H25···O3^{vii}	0.93	2.37	3.238 (8)	154

Symmetry codes: (v) −*x*+1/2, −*y*+3/2, −*z*; (vi) *x*+1/2, −*y*+3/2, *z*+1/2; (vii) *x*, *y*−1, *z*.