catena-Poly[[(4,7-diphenyl-1,10-phenanthroline)cadmium(II)]-μ-4,4'-oxydibenzoato]

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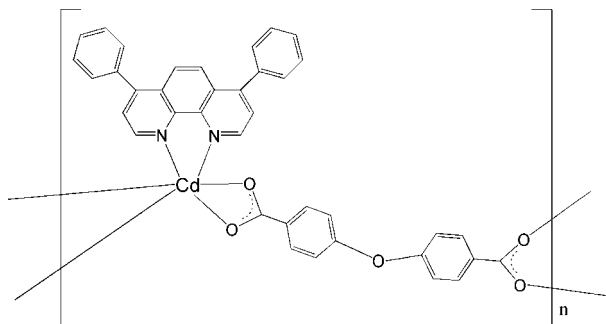
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In the title compound, $[Cd(C_{14}H_8O_5)(C_{24}H_{16}N_2)]_n$, the Cd^{II} atom is chelated by 4,7-diphenyl-1,10-phenanthroline (*L*) and is also bonded to four O atoms from three different 4,4'-oxydibenzoate (oba) ligands, resulting in a distorted *cis*-CdN_2O_4 octahedral geometry. The oba ligands bridge neighbouring Cd^{II} atoms, generating a chain structure. Aromatic π–π stacking between *L* ligands in adjacent chains leads to a two-dimensional supramolecular layer [minimum centroid–centroid separation = 3.453 (6) Å].

Related literature

For studies of related Cd^{II} coordination polymers, see: Chen & Liu (2002).

Experimental

Crystal data

$[Cd(C_{14}H_8O_5)(C_{24}H_{16}N_2)]$	γ = 96.34 (3)°
M_r = 700.99	V = 1480.0 (5) Å³
Triclinic, $P\bar{1}$	Z = 2
a = 10.727 (2) Å	Mo $K\alpha$ radiation
b = 10.960 (2) Å	μ = 0.79 mm⁻¹
c = 13.375 (3) Å	T = 293 (2) K
α = 92.85 (3)°	0.31 × 0.22 × 0.21 mm
β = 108.06 (3)°	

Data collection

Rigaku R-AXIS RAPID diffractometer	14656 measured reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	6675 independent reflections
T_{min} = 0.778, T_{max} = 0.846	5903 reflections with $I > 2\sigma(I)$
	R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029	415 parameters
$wR(F^2)$ = 0.078	H-atom parameters constrained
S = 1.17	$\Delta\rho_{max}$ = 0.45 e Å⁻³
6675 reflections	$\Delta\rho_{min}$ = −0.40 e Å⁻³

Table 1
Selected bond lengths (Å).

Cd1—N1	2.4010 (19)	Cd1—O2	2.457 (2)
Cd1—N2	2.3474 (19)	Cd1—O4^i	2.2749 (19)
Cd1—O1	2.372 (2)	Cd1—O5^{ii}	2.2389 (19)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2643).

References

Chen, X.-M. & Liu, G.-F. (2002). *Chem. Eur. J.* **8**, 4811–4817.
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Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan. (1998).
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supplementary materials

catena-Poly[[(4,7-diphenyl-1,10-phenanthroline)cadmium(II)]-$^\mu$-4,4'-oxydibenzoato]

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Comment

1,10-Phenanthroline (phen) has been widely used in the construction of metal-organic coordination polymers (Chen & Liu, 2002). However, 4,7-diphenyl-1,10-phenanthroline (*L*), as a derivative of phen, has received less attention as a ligand. Herein, we present a new Cd(II) coordination polymer, namely the title compound, (I), [Cd(oba)(*L*)], where oba =4,4'-oxybis(benzate) and *L* = 4,7-diphenyl-1,10-phenanthroline.

In compound (I) the Cd^{II} atom is six-coordinated by four carboxylate O atoms from three different oba ligands and two N atoms from one *L* ligand (Table 1, Fig. 1). The neighboring Cd^{II} atoms are linked by the oba dianions to form an interesting chain structure. The *L* ligands are decorded on both sides of the chains (Fig. 2). Furthermore, the π-π interactions between *L* ligands in neighboring chains result in a two-dimensional supramolecular layer structure [minimum centroid-centroid separation = 3.453 (6) Å].

Experimental

A mixture of Cd(NO$_3$)$_2$·4H$_2$O (1 mmol), H$_2$oba (1 mmol) and *L* (1 mmol) were dissolved in 15 ml distilled water, followed by addition of triethylamine until the pH value of the system was adjusted to about 6.0. The resulting solution was sealed in a 23-ml Teflon-lined stainless steel autoclave and heated at 445 K for 3 days under autogenous pressure. Afterwards, the reaction system was slowly cooled to room temperature. Colourless blocks of (I) were collected.

Refinement

All the H atoms were generated geometrically (C—H = 0.93 Å) and refined as riding with U_{iso}(H)= $1.2U_{eq}$(C).
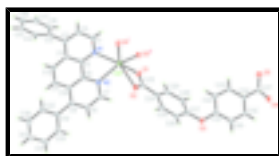
Figures

Fig. 1. The asymmetric unit of (I) expanded to show the cadmium coordination sphere, with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. H atoms omitted for clarity. Symmetry codes: (i) $x, y, z − 1$; (ii) $1 − x, 1 − y, 2 − z$.
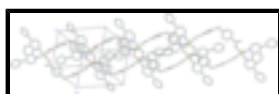

Fig. 2. View of the chain structure of (I). The hydrogen atoms are omitted for clarity.

supplementary materials

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Crystal data

$[Cd(C_{14}H_8O_5)(C_{24}H_{16}N_2)]$	$Z = 2$
$M_r = 700.99$	$F_{000} = 708$
Triclinic, $P\bar{1}$	$D_x = 1.573$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.727\ (2)$ Å	Cell parameters from 13489 reflections
$b = 10.960\ (2)$ Å	$\theta = 3.0–27.5º$
$c = 13.375\ (3)$ Å	$\mu = 0.79$ mm^{-1}
$\alpha = 92.85\ (3)º$	$T = 293\ (2)$ K
$\beta = 108.06\ (3)º$	Block, colorless
$\gamma = 96.34\ (3)º$	$0.31 \times 0.22 \times 0.21$ mm
$V = 1480.0\ (5)$ Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	6675 independent reflections
Radiation source: rotating anode	5903 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
Detector resolution: 10.0 pixels mm^{-1}	$\theta_{max} = 27.5º$
$T = 293(2)$ K	$\theta_{min} = 3.2º$
ω scan	$h = -13 \rightarrow 13$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -14 \rightarrow 14$
$T_{min} = 0.778$, $T_{max} = 0.846$	$l = -17 \rightarrow 17$
14656 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
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.078$	$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.263P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} = 0.002$
6675 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
415 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.6637 (2)	0.6060 (2)	0.37389 (18)	0.0332 (5)
H1	0.6025	0.6403	0.3992	0.040*
C2	0.6826 (2)	0.6458 (2)	0.28126 (19)	0.0372 (5)
H2	0.6325	0.7038	0.2458	0.045*
C3	0.7738 (2)	0.6007 (2)	0.24197 (18)	0.0318 (5)
C4	0.8459 (2)	0.5097 (2)	0.29766 (16)	0.0275 (4)
C5	0.81712 (19)	0.4713 (2)	0.38772 (16)	0.0253 (4)
C6	0.88064 (19)	0.3725 (2)	0.44245 (16)	0.0253 (4)
C7	0.9048 (2)	0.2453 (2)	0.57706 (19)	0.0371 (5)
H7	0.8858	0.2229	0.6374	0.045*
C8	0.9903 (2)	0.1811 (2)	0.54251 (19)	0.0369 (5)
H8	1.0253	0.1161	0.5788	0.044*
C9	1.0240 (2)	0.2131 (2)	0.45465 (17)	0.0308 (5)
C10	0.97134 (19)	0.3157 (2)	0.40378 (16)	0.0267 (4)
C11	1.0081 (2)	0.3666 (2)	0.31927 (17)	0.0301 (4)
H11	1.0743	0.3356	0.2983	0.036*
C12	0.9485 (2)	0.4592 (2)	0.26896 (17)	0.0299 (4)
H12	0.9750	0.4907	0.2144	0.036*
C13	0.7934 (2)	0.6468 (2)	0.14384 (18)	0.0349 (5)
C14	0.7898 (3)	0.5666 (3)	0.05885 (19)	0.0412 (6)
H14	0.7792	0.4820	0.0639	0.049*
C15	0.8017 (3)	0.6114 (3)	−0.0337 (2)	0.0512 (7)
H15	0.7994	0.5569	−0.0900	0.061*
C16	0.8167 (3)	0.7360 (3)	−0.0418 (2)	0.0557 (8)
H16	0.8234	0.7657	−0.1041	0.067*
C17	0.8220 (3)	0.8167 (3)	0.0410 (3)	0.0614 (8)
H17	0.8343	0.9012	0.0355	0.074*
C18	0.8088 (3)	0.7724 (3)	0.1345 (2)	0.0504 (7)
H18	0.8104	0.8276	0.1901	0.061*
C19	1.1120 (2)	0.1413 (2)	0.4157 (2)	0.0361 (5)
C20	1.2313 (3)	0.1185 (2)	0.4854 (2)	0.0439 (6)
H20	1.2549	0.1472	0.5563	0.053*
C21	1.3154 (3)	0.0535 (3)	0.4503 (3)	0.0588 (8)

H21	1.3956	0.0395	0.4975	0.071*
C22	1.0767 (3)	0.0942 (3)	0.3104 (2)	0.0471 (6)
H22	0.9963	0.1071	0.2628	0.056*
C23	0.7171 (2)	0.3036 (2)	0.75097 (18)	0.0351 (5)
C24	0.7178 (2)	0.2417 (2)	0.84919 (17)	0.0307 (5)
C25	0.8257 (2)	0.2671 (3)	0.9397 (2)	0.0407 (6)
H25	0.9009	0.3168	0.9379	0.049*
C26	0.8232 (3)	0.2194 (3)	1.0335 (2)	0.0436 (6)
H26	0.8966	0.2353	1.0940	0.052*
C27	0.7100 (3)	0.1480 (2)	1.03528 (19)	0.0380 (5)
C28	0.6038 (3)	0.1172 (3)	0.9450 (2)	0.0458 (6)
H28	0.5299	0.0652	0.9465	0.055*
C29	0.6081 (2)	0.1646 (2)	0.85146 (19)	0.0391 (5)
H29	0.5366	0.1443	0.7901	0.047*
C31	0.6376 (2)	0.1703 (2)	1.18442 (18)	0.0345 (5)
C32	0.5706 (3)	0.2679 (3)	1.14457 (18)	0.0397 (6)
H32	0.5706	0.2943	1.0796	0.048*
C33	0.5040 (2)	0.3251 (2)	1.20322 (17)	0.0355 (5)
H33	0.4566	0.3885	1.1758	0.043*
C34	0.5063 (2)	0.2900 (2)	1.30192 (17)	0.0322 (5)
C35	0.5775 (2)	0.1941 (2)	1.34149 (17)	0.0352 (5)
H35	0.5822	0.1707	1.4083	0.042*
C36	0.6408 (2)	0.1339 (2)	1.28275 (18)	0.0367 (5)
H36	0.6858	0.0686	1.3091	0.044*
C37	0.4414 (2)	0.3591 (2)	1.36633 (18)	0.0337 (5)
C38	1.1620 (4)	0.0279 (3)	0.2767 (3)	0.0639 (9)
H38	1.1381	−0.0041	0.2067	0.077*
C30	1.2814 (4)	0.0098 (3)	0.3466 (3)	0.0674 (10)
H30	1.3392	−0.0324	0.3232	0.081*
N1	0.72926 (17)	0.52138 (18)	0.42724 (14)	0.0282 (4)
N2	0.84895 (18)	0.33720 (18)	0.52780 (14)	0.0307 (4)
O1	0.61682 (18)	0.27675 (19)	0.66971 (14)	0.0464 (4)
O2	0.81336 (18)	0.3792 (2)	0.75375 (15)	0.0480 (5)
O3	0.7058 (2)	0.10611 (19)	1.13135 (14)	0.0493 (5)
O4	0.48556 (16)	0.3603 (2)	1.46570 (13)	0.0450 (4)
O5	0.34624 (19)	0.41474 (19)	1.31991 (14)	0.0474 (5)
Cd1	0.690321 (14)	0.434330 (16)	0.577806 (12)	0.02952 (6)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0311 (11)	0.0373 (13)	0.0375 (12)	0.0104 (9)	0.0178 (10)	0.0033 (9)
C2	0.0373 (12)	0.0384 (14)	0.0404 (12)	0.0150 (10)	0.0143 (10)	0.0103 (10)
C3	0.0339 (11)	0.0305 (12)	0.0323 (11)	0.0065 (9)	0.0114 (9)	0.0047 (9)
C4	0.0272 (10)	0.0270 (11)	0.0287 (10)	0.0036 (8)	0.0094 (9)	0.0018 (8)
C5	0.0231 (9)	0.0281 (11)	0.0265 (9)	0.0034 (8)	0.0107 (8)	0.0007 (8)
C6	0.0237 (9)	0.0279 (11)	0.0257 (9)	0.0029 (8)	0.0101 (8)	0.0018 (8)
C7	0.0424 (13)	0.0401 (14)	0.0356 (12)	0.0113 (10)	0.0189 (10)	0.0111 (10)

C8	0.0446 (13)	0.0344 (13)	0.0382 (12)	0.0133 (10)	0.0187 (11)	0.0115 (10)
C9	0.0315 (11)	0.0301 (12)	0.0342 (11)	0.0069 (9)	0.0141 (9)	0.0034 (9)
C10	0.0249 (9)	0.0288 (11)	0.0287 (10)	0.0041 (8)	0.0121 (8)	0.0014 (8)
C11	0.0279 (10)	0.0336 (12)	0.0324 (11)	0.0063 (8)	0.0141 (9)	0.0026 (9)
C12	0.0314 (10)	0.0333 (12)	0.0301 (10)	0.0048 (9)	0.0164 (9)	0.0060 (9)
C13	0.0356 (11)	0.0417 (14)	0.0326 (11)	0.0110 (10)	0.0148 (10)	0.0116 (10)
C14	0.0438 (13)	0.0448 (15)	0.0367 (12)	0.0090 (11)	0.0134 (11)	0.0087 (11)
C15	0.0481 (15)	0.077 (2)	0.0320 (12)	0.0143 (14)	0.0153 (12)	0.0093 (13)
C16	0.0513 (16)	0.080 (2)	0.0459 (15)	0.0166 (15)	0.0236 (13)	0.0304 (15)
C17	0.072 (2)	0.0528 (19)	0.068 (2)	0.0146 (15)	0.0290 (17)	0.0319 (16)
C18	0.0645 (17)	0.0431 (16)	0.0514 (15)	0.0153 (13)	0.0254 (14)	0.0130 (12)
C19	0.0440 (12)	0.0289 (12)	0.0447 (13)	0.0120 (10)	0.0241 (11)	0.0085 (10)
C20	0.0424 (13)	0.0369 (14)	0.0585 (16)	0.0131 (11)	0.0220 (12)	0.0045 (12)
C21	0.0489 (16)	0.0433 (17)	0.095 (2)	0.0206 (13)	0.0325 (17)	0.0098 (16)
C22	0.0641 (17)	0.0409 (15)	0.0445 (14)	0.0147 (13)	0.0262 (13)	0.0062 (11)
C23	0.0428 (13)	0.0377 (13)	0.0349 (12)	0.0151 (10)	0.0228 (11)	0.0093 (10)
C24	0.0365 (11)	0.0326 (12)	0.0307 (11)	0.0101 (9)	0.0194 (9)	0.0049 (9)
C25	0.0397 (13)	0.0473 (15)	0.0390 (13)	0.0043 (11)	0.0177 (11)	0.0095 (11)
C26	0.0470 (14)	0.0521 (16)	0.0319 (12)	0.0119 (12)	0.0108 (11)	0.0052 (11)
C27	0.0548 (14)	0.0390 (14)	0.0339 (11)	0.0196 (11)	0.0282 (11)	0.0098 (10)
C28	0.0497 (14)	0.0494 (16)	0.0463 (14)	0.0012 (12)	0.0271 (12)	0.0138 (12)
C29	0.0421 (13)	0.0414 (14)	0.0354 (12)	0.0032 (10)	0.0152 (11)	0.0049 (10)
C31	0.0400 (12)	0.0388 (14)	0.0312 (11)	0.0090 (10)	0.0189 (10)	0.0050 (9)
C32	0.0517 (14)	0.0477 (15)	0.0270 (11)	0.0161 (11)	0.0186 (11)	0.0112 (10)
C33	0.0386 (12)	0.0431 (14)	0.0266 (10)	0.0128 (10)	0.0101 (9)	0.0055 (9)
C34	0.0304 (11)	0.0381 (13)	0.0260 (10)	0.0012 (9)	0.0078 (9)	−0.0012 (9)
C35	0.0415 (12)	0.0411 (14)	0.0260 (10)	0.0048 (10)	0.0144 (10)	0.0077 (9)
C36	0.0442 (13)	0.0377 (13)	0.0322 (11)	0.0098 (10)	0.0153 (10)	0.0115 (10)
C37	0.0301 (11)	0.0415 (14)	0.0306 (11)	−0.0010 (9)	0.0140 (9)	−0.0037 (9)
C38	0.105 (3)	0.0408 (17)	0.0654 (19)	0.0168 (17)	0.053 (2)	−0.0001 (14)
C30	0.077 (2)	0.0454 (18)	0.109 (3)	0.0214 (16)	0.067 (2)	0.0075 (18)
N1	0.0249 (8)	0.0327 (10)	0.0303 (9)	0.0062 (7)	0.0127 (7)	0.0027 (7)
N2	0.0318 (9)	0.0364 (11)	0.0282 (9)	0.0079 (8)	0.0143 (8)	0.0058 (8)
O1	0.0489 (10)	0.0551 (12)	0.0355 (9)	0.0089 (9)	0.0115 (8)	0.0141 (8)
O2	0.0461 (10)	0.0614 (13)	0.0440 (10)	0.0013 (9)	0.0251 (9)	0.0168 (9)
O3	0.0764 (13)	0.0522 (12)	0.0389 (9)	0.0323 (10)	0.0360 (9)	0.0200 (8)
O4	0.0356 (9)	0.0728 (14)	0.0276 (8)	0.0002 (8)	0.0149 (7)	−0.0028 (8)
O5	0.0520 (11)	0.0571 (12)	0.0367 (9)	0.0212 (9)	0.0155 (8)	−0.0020 (8)
Cd1	0.02898 (9)	0.03929 (11)	0.02562 (9)	0.00848 (6)	0.01462 (6)	0.00524 (6)

Geometric parameters (Å, °)

C1—N1	1.328 (3)	C22—C38	1.392 (4)
C1—C2	1.399 (3)	C22—H22	0.9300
C1—H1	0.9300	C23—O2	1.241 (3)
C2—C3	1.371 (3)	C23—O1	1.264 (3)
C2—H2	0.9300	C23—C24	1.506 (3)
C3—C4	1.426 (3)	C23—Cd1	2.740 (2)
C3—C13	1.495 (3)	C24—C29	1.380 (3)

C4—C5	1.406 (3)	C24—C25	1.382 (4)
C4—C12	1.428 (3)	C25—C26	1.390 (3)
C5—N1	1.365 (3)	C25—H25	0.9300
C5—C6	1.451 (3)	C26—C27	1.377 (4)
C6—N2	1.350 (3)	C26—H26	0.9300
C6—C10	1.419 (3)	C27—C28	1.376 (4)
C7—N2	1.328 (3)	C27—O3	1.398 (3)
C7—C8	1.386 (3)	C28—C29	1.390 (3)
C7—H7	0.9300	C28—H28	0.9300
C8—C9	1.382 (3)	C29—H29	0.9300
C8—H8	0.9300	C31—C36	1.385 (3)
C9—C10	1.424 (3)	C31—O3	1.386 (3)
C9—C19	1.485 (3)	C31—C32	1.390 (3)
C10—C11	1.426 (3)	C32—C33	1.384 (3)
C11—C12	1.356 (3)	C32—H32	0.9300
C11—H11	0.9300	C33—C34	1.387 (3)
C12—H12	0.9300	C33—H33	0.9300
C13—C18	1.385 (4)	C34—C35	1.397 (3)
C13—C14	1.390 (4)	C34—C37	1.491 (3)
C14—C15	1.390 (4)	C35—C36	1.375 (3)
C14—H14	0.9300	C35—H35	0.9300
C15—C16	1.371 (5)	C36—H36	0.9300
C15—H15	0.9300	C37—O5	1.258 (3)
C16—C17	1.366 (5)	C37—O4	1.264 (3)
C16—H16	0.9300	C38—C30	1.373 (5)
C17—C18	1.404 (4)	C38—H38	0.9300
C17—H17	0.9300	C30—H30	0.9300
C18—H18	0.9300	Cd1—N1	2.4010 (19)
C19—C20	1.387 (4)	Cd1—N2	2.3474 (19)
C19—C22	1.396 (4)	Cd1—O1	2.372 (2)
C20—C21	1.384 (4)	Cd1—O2	2.457 (2)
C20—H20	0.9300	Cd1—O4[i]	2.2749 (19)
C21—C30	1.367 (5)	Cd1—O5[ii]	2.2389 (19)
C21—H21	0.9300		
N1—C1—C2	122.8 (2)	C29—C24—C25	119.4 (2)
N1—C1—H1	118.6	C29—C24—C23	120.4 (2)
C2—C1—H1	118.6	C25—C24—C23	120.1 (2)
C3—C2—C1	121.0 (2)	C24—C25—C26	120.8 (2)
C3—C2—H2	119.5	C24—C25—H25	119.6
C1—C2—H2	119.5	C26—C25—H25	119.6
C2—C3—C4	117.4 (2)	C27—C26—C25	118.8 (2)
C2—C3—C13	119.7 (2)	C27—C26—H26	120.6
C4—C3—C13	122.9 (2)	C25—C26—H26	120.6
C5—C4—C3	117.90 (19)	C28—C27—C26	121.2 (2)
C5—C4—C12	118.55 (19)	C28—C27—O3	120.4 (2)
C3—C4—C12	123.5 (2)	C26—C27—O3	118.3 (2)
N1—C5—C4	123.26 (19)	C27—C28—C29	119.3 (2)
N1—C5—C6	116.80 (18)	C27—C28—H28	120.3

C4—C5—C6	119.93 (18)	C29—C28—H28	120.3
N2—C6—C10	122.72 (19)	C24—C29—C28	120.3 (2)
N2—C6—C5	118.09 (18)	C24—C29—H29	119.8
C10—C6—C5	119.19 (18)	C28—C29—H29	119.8
N2—C7—C8	122.9 (2)	C36—C31—O3	116.4 (2)
N2—C7—H7	118.5	C36—C31—C32	120.2 (2)
C8—C7—H7	118.5	O3—C31—C32	123.4 (2)
C9—C8—C7	120.6 (2)	C33—C32—C31	118.9 (2)
C9—C8—H8	119.7	C33—C32—H32	120.5
C7—C8—H8	119.7	C31—C32—H32	120.5
C8—C9—C10	117.7 (2)	C32—C33—C34	121.6 (2)
C8—C9—C19	120.4 (2)	C32—C33—H33	119.2
C10—C9—C19	122.0 (2)	C34—C33—H33	119.2
C6—C10—C9	117.57 (19)	C33—C34—C35	118.3 (2)
C6—C10—C11	118.70 (19)	C33—C34—C37	120.3 (2)
C9—C10—C11	123.70 (19)	C35—C34—C37	121.3 (2)
C12—C11—C10	121.3 (2)	C36—C35—C34	120.7 (2)
C12—C11—H11	119.4	C36—C35—H35	119.6
C10—C11—H11	119.4	C34—C35—H35	119.6
C11—C12—C4	121.7 (2)	C35—C36—C31	120.1 (2)
C11—C12—H12	119.2	C35—C36—H36	119.9
C4—C12—H12	119.2	C31—C36—H36	119.9
C18—C13—C14	118.6 (2)	O5—C37—O4	122.7 (2)
C18—C13—C3	119.6 (2)	O5—C37—C34	118.9 (2)
C14—C13—C3	121.7 (2)	O4—C37—C34	118.4 (2)
C13—C14—C15	120.8 (3)	C30—C38—C22	120.2 (3)
C13—C14—H14	119.6	C30—C38—H38	119.9
C15—C14—H14	119.6	C22—C38—H38	119.9
C16—C15—C14	119.9 (3)	C21—C30—C38	120.2 (3)
C16—C15—H15	120.1	C21—C30—H30	119.9
C14—C15—H15	120.1	C38—C30—H30	119.9
C17—C16—C15	120.5 (3)	C1—N1—C5	117.48 (18)
C17—C16—H16	119.8	C1—N1—Cd1	125.23 (14)
C15—C16—H16	119.8	C5—N1—Cd1	116.98 (14)
C16—C17—C18	120.1 (3)	C7—N2—C6	118.40 (19)
C16—C17—H17	120.0	C7—N2—Cd1	122.82 (15)
C18—C17—H17	120.0	C6—N2—Cd1	118.71 (14)
C13—C18—C17	120.1 (3)	C23—O1—Cd1	92.71 (15)
C13—C18—H18	119.9	C23—O2—Cd1	89.37 (15)
C17—C18—H18	119.9	C31—O3—C27	116.40 (18)
C20—C19—C22	118.8 (2)	C37—O4—Cd1^{iii}	129.23 (15)
C20—C19—C9	119.6 (2)	C37—O5—Cd1^{ii}	113.88 (15)
C22—C19—C9	121.6 (2)	O5^{ii}—Cd1—O4^{i}	104.08 (7)
C21—C20—C19	120.5 (3)	O5^{ii}—Cd1—N2	146.36 (7)
C21—C20—H20	119.8	O4^{i}—Cd1—N2	109.10 (7)
C19—C20—H20	119.8	O5^{ii}—Cd1—O1	93.21 (7)
C30—C21—C20	120.4 (3)	O4^{i}—Cd1—O1	77.24 (7)

C30—C21—H21	119.8	N2—Cd1—O1	99.27 (7)
C20—C21—H21	119.8	O5^{ii}—Cd1—N1	108.40 (7)
C38—C22—C19	119.9 (3)	O4^{i}—Cd1—N1	85.70 (7)
C38—C22—H22	120.0	N2—Cd1—N1	69.37 (7)
C19—C22—H22	120.0	O1—Cd1—N1	155.25 (7)
O2—C23—O1	123.1 (2)	O5^{ii}—Cd1—O2	79.43 (7)
O2—C23—C24	118.9 (2)	O4^{i}—Cd1—O2	131.45 (7)
O1—C23—C24	118.0 (2)	N2—Cd1—O2	82.82 (7)
O2—C23—Cd1	63.71 (13)	O1—Cd1—O2	54.25 (7)
O1—C23—Cd1	59.85 (13)	N1—Cd1—O2	140.14 (6)
C24—C23—Cd1	172.07 (15)		

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

Fig. 1

Fig. 2