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catena-Poly[[(1,10-phenanthroline-κ^2N,N')(pyridine-3-carboxylato-$\kappa^2O:O'$)cadmium(II)]-μ-pyridine-3-carboxylato-$\kappa^3N:O,O'$]

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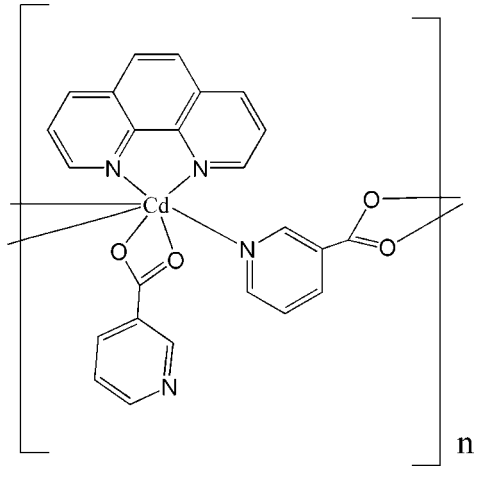
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.058; data-to-parameter ratio = 15.7.

The title complex, $[Cd(C_6H_4NO_2)_2(C_{12}H_8N_2)]_n$, is a one-dimensional chain-like coordination polymer. Adjacent chains are further aggregated into a three-dimensional network through π–π (interplanar distance is 3.5806 Å) and C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Chen *et al.* (2003); Gerrard & Wood (2000); Gutschke *et al.* (1995); Leininger *et al.* (2000); Li *et al.* (2006); Swiegers & Malefetse (2000); Yu *et al.* (2004).



Experimental

Crystal data

$[Cd(C_6H_4NO_2)_2(C_{12}H_8N_2)]$
M_r = 536.81
Triclinic, $P\overline{1}$
a = 7.9274 (5) Å
b = 10.8456 (7) Å
c = 13.3381 (9) Å
α = 77.705 (1)°
β = 84.094 (1)°
γ = 69.984 (1)°
V = 1052.23 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 293 (2) K
0.41 × 0.26 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.666, T_{max} = 0.882
6811 measured reflections
4681 independent reflections
4465 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.058
S = 1.07
4681 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

*Cg*1 is the centroid of the N2/C7–C11 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots Cg1^{i}$	0.93	2.97	3.853 (2)	158
C17—H17$\cdots Cg1^{ii}$	0.93	2.67	3.435 (2)	140

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2189).

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supplementary materials

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catena-Poly[[(1,10-phenanthroline-κ^2N,N')(pyridine-3-carboxylato-$\kappa^2O:O'$)cadmium(II)]-μ-pyridine-3-carboxylato-$\kappa^3N:O,O'$]

H.-C. Yi and P. Mei

Comment

Metal-organic coordination polymers have attracted considerable attention due to their intriguing potential applications, such as catalysis, magnetism, electronic and chemical separation (Leininger *et al.*, 2000; Swiegers *et al.*, 2000). Polydentate organic ligands are an important kind of ligands to construct coordination polymers. Many these hybrid materials have been synthesized and characterized by rational selection of suitable ligands. Among the various ligands, multidentate N– or O-donor ligands, such as pyridine- or imidazole-(di)carboxylic acids, have drawn extensive attention in the construction of coordination polymer. Pyridine-2,3-dicarboxylic acid is ralely used a linkage ligand (Gutschke *et al.*, 1995; Yu *et al.*, 2004). We present here the title new coordination polymer, (I), in which pyridine-2,3-dicarboxylic acid decarboxylates one carboxylic group and transforms to pyridine-3-carboxylic acid.

Compound (I) is a one-dimensional (one-dimensional) chain-like coordination polymer. The Cd^{II} ion of (I) is seven-coordinated by two N atoms from 1,10-phenanthroline, one N atoms and four O atoms from three different pyridine-3-dicarboxylates (Fig. 1). There are two types of pyridine-3-dicarboxylates, one chelating Cd^{II} with carboxylates, and the other acting as a bridge ligand with N atoms and carboxylates. The latter ligand link Cd^{II} ions to form a one-dimensional chain along *a* axis. Two adjacent chains are linked together *via* π-π interactions between the N3,C13,C14,C15,C16,C24 and N4,C22, C21,C20,C19,C23 rings of the 1,10-phenanthroline ligands with plane-to-plane distances of 3.542 and 3.565 Å and a slippage of 1.143 Å and 0.955 Å respectively. The dimeric chains further extend to three-dimensional (three-dimensional) supramolecular structure *via* π-π interactions between pyridine rings with a distance of 3.555 Å and a slippage of 0.427 Å. The whole packing is further stabilized by weak C—H···π interactions (Table 1).

Experimental

A mixture of CdO (0.064 g, 0.05 mmol), 1,10-phenanthroline (0.0198 g, 0.1 mmol), pyridine-2,3-dicarboxylic acid (0.0167 g, 0.1 mmol) and 5.0 ml distilled water was mixed in a Teflon-lined autoclave and heated at 393 K for 3 days. After cooled to room temperature, block-like colorless crystals of (I) were obtained and washed with distlled water. The pyridine-3-dicarboxylic acid in (I) was believed to be obtained from *in situ* decarboxylation of pyridine-2,3-dicarboxylic acid. The similar decomposing behaviors have been observed previously (Gerrard, *et al.* 2000; Chen, *et al.* 2003; Li, *et al.* 2006)

Refinement

Hydrogen atoms bonded to C atoms were placed in idealized location, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

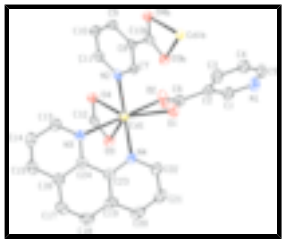


Fig. 1. The coordination environment of Cd in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. All H atoms have been omitted for clarify.

catena-Poly[[(1,10-phenanthroline-κ^2*N*,*N*')(pyridine-3-carboxylato-\ κ^2*O*:*O*')cadmium(II)]-μ-pyridine-3-carboxylato-κ^3*N*:*O*,*O*']

Crystal data

$[Cd(C_6H_4NO_2)_2(C_{12}H_8N_2)]$	$Z = 2$
$M_r = 536.81$	$F_{000} = 536$
Triclinic, $P\overline{1}$	$D_x = 1.694$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.9274$ (5) Å	Cell parameters from 5362 reflections
$b = 10.8456$ (7) Å	$\theta = 2.3$–29.5º
$c = 13.3381$ (9) Å	$\mu = 1.08$ mm^{-1}
$\alpha = 77.705$ (1)º	$T = 293$ (2) K
$\beta = 84.094$ (1)º	Block, colourless
$\gamma = 69.984$ (1)º	0.41 × 0.26 × 0.12 mm
$V = 1052.23$ (12) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4681 independent reflections
Radiation source: fine-focus sealed tube	4465 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 293$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -9 \rightarrow 10$
$T_{min} = 0.666$, $T_{max} = 0.882$	$k = -11 \rightarrow 14$
6811 measured reflections	$l = -17 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained

$wR(F^2) = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0261P)^2 + 0.3996P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
4681 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.51$ 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}
Cd1	0.781715 (17)	0.224799 (13)	0.236286 (10)	0.03447 (5)
C1	0.9019 (3)	0.6148 (2)	0.33832 (19)	0.0525 (5)
H1	0.9584	0.6033	0.2747	0.063*
C2	0.8012 (3)	0.5342 (2)	0.38131 (17)	0.0437 (5)
C3	0.7195 (3)	0.5516 (2)	0.4763 (2)	0.0545 (6)
H3	0.6496	0.5000	0.5084	0.065*
C4	0.7429 (4)	0.6465 (2)	0.5229 (2)	0.0586 (6)
H4	0.6900	0.6598	0.5870	0.070*
C5	0.8461 (4)	0.7207 (2)	0.4721 (2)	0.0575 (6)
H5	0.8617	0.7842	0.5040	0.069*
C6	0.7872 (3)	0.4299 (2)	0.3280 (2)	0.0529 (6)
C7	1.1925 (2)	0.14076 (18)	0.29063 (14)	0.0320 (4)
H7	1.1776	0.2225	0.2467	0.038*
C8	1.3578 (2)	0.07150 (18)	0.33359 (13)	0.0301 (3)
C9	1.3781 (3)	−0.0484 (2)	0.40090 (15)	0.0375 (4)
H9	1.4867	−0.0961	0.4326	0.045*
C10	1.2348 (3)	−0.0964 (2)	0.42046 (16)	0.0436 (5)
H10	1.2457	−0.1772	0.4649	0.052*
C11	1.0757 (3)	−0.0219 (2)	0.37277 (16)	0.0405 (4)
H11	0.9800	−0.0548	0.3853	0.049*
C12	1.5107 (2)	0.12578 (19)	0.30540 (14)	0.0325 (4)
C13	0.8300 (3)	−0.0623 (2)	0.14946 (18)	0.0495 (5)
H13	0.8667	−0.1050	0.2156	0.059*
C14	0.7972 (4)	−0.1364 (2)	0.0844 (2)	0.0606 (6)
H14	0.8126	−0.2267	0.1069	0.073*

C15	0.7424 (4)	−0.0746 (3)	−0.0124 (2)	0.0620 (7)
H15	0.7183	−0.1222	−0.0562	0.074*
C16	0.7224 (3)	0.0611 (2)	−0.04569 (17)	0.0502 (5)
C17	0.6681 (4)	0.1327 (3)	−0.14689 (19)	0.0654 (7)
H17	0.6410	0.0888	−0.1926	0.078*
C18	0.6558 (4)	0.2608 (3)	−0.17691 (19)	0.0661 (7)
H18	0.6224	0.3042	−0.2435	0.079*
C19	0.6929 (3)	0.3319 (2)	−0.10875 (17)	0.0504 (5)
C20	0.6834 (4)	0.4663 (3)	−0.13723 (19)	0.0624 (7)
H20	0.6527	0.5127	−0.2035	0.075*
C21	0.7189 (4)	0.5282 (3)	−0.0683 (2)	0.0657 (7)
H21	0.7138	0.6171	−0.0868	0.079*
C22	0.7633 (4)	0.4577 (2)	0.03071 (19)	0.0557 (6)
H22	0.7872	0.5016	0.0775	0.067*
C23	0.7411 (3)	0.2671 (2)	−0.00733 (15)	0.0402 (4)
C24	0.7590 (3)	0.1274 (2)	0.02443 (15)	0.0386 (4)
N1	0.9242 (3)	0.7081 (2)	0.38144 (18)	0.0617 (5)
N2	1.0527 (2)	0.09557 (16)	0.30935 (12)	0.0352 (3)
N3	0.8111 (2)	0.06612 (17)	0.12083 (13)	0.0399 (4)
N4	0.7732 (2)	0.33079 (17)	0.06161 (13)	0.0421 (4)
O1	0.8802 (3)	0.41230 (19)	0.24723 (15)	0.0697 (5)
O2	0.6869 (3)	0.3643 (2)	0.36485 (19)	0.0807 (6)
O3	1.48444 (19)	0.22957 (14)	0.23695 (12)	0.0451 (3)
O4	1.65543 (18)	0.06529 (15)	0.34869 (11)	0.0428 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02902 (8)	0.03845 (8)	0.03973 (8)	−0.01887 (6)	−0.00330 (5)	−0.00146 (6)
C1	0.0635 (15)	0.0442 (12)	0.0508 (12)	−0.0217 (11)	0.0034 (11)	−0.0072 (10)
C2	0.0437 (11)	0.0358 (10)	0.0508 (12)	−0.0111 (8)	−0.0074 (9)	−0.0068 (8)
C3	0.0559 (14)	0.0493 (13)	0.0618 (14)	−0.0248 (11)	0.0070 (11)	−0.0099 (11)
C4	0.0729 (17)	0.0507 (13)	0.0503 (13)	−0.0173 (12)	0.0040 (12)	−0.0136 (10)
C5	0.0745 (17)	0.0449 (12)	0.0598 (14)	−0.0249 (12)	−0.0057 (12)	−0.0138 (11)
C6	0.0565 (14)	0.0403 (11)	0.0625 (15)	−0.0108 (10)	−0.0163 (11)	−0.0123 (10)
C7	0.0301 (9)	0.0342 (9)	0.0356 (9)	−0.0167 (7)	−0.0027 (7)	−0.0040 (7)
C8	0.0293 (8)	0.0353 (9)	0.0312 (8)	−0.0168 (7)	−0.0009 (6)	−0.0075 (7)
C9	0.0331 (9)	0.0426 (10)	0.0382 (10)	−0.0167 (8)	−0.0077 (7)	−0.0002 (8)
C10	0.0447 (11)	0.0433 (11)	0.0445 (11)	−0.0241 (9)	−0.0063 (9)	0.0063 (8)
C11	0.0372 (10)	0.0461 (11)	0.0456 (10)	−0.0274 (8)	−0.0018 (8)	−0.0013 (8)
C12	0.0278 (9)	0.0387 (9)	0.0367 (9)	−0.0169 (7)	0.0009 (7)	−0.0101 (7)
C13	0.0540 (13)	0.0434 (11)	0.0502 (12)	−0.0182 (10)	0.0008 (10)	−0.0041 (9)
C14	0.0740 (18)	0.0438 (13)	0.0674 (16)	−0.0235 (12)	0.0069 (13)	−0.0150 (11)
C15	0.0754 (18)	0.0584 (15)	0.0611 (15)	−0.0255 (13)	0.0054 (13)	−0.0279 (12)
C16	0.0516 (13)	0.0528 (13)	0.0458 (12)	−0.0133 (10)	0.0012 (10)	−0.0162 (10)
C17	0.0823 (19)	0.0722 (17)	0.0438 (13)	−0.0195 (14)	−0.0072 (12)	−0.0231 (12)
C18	0.0807 (19)	0.0696 (17)	0.0377 (12)	−0.0101 (14)	−0.0088 (12)	−0.0091 (11)
C19	0.0505 (13)	0.0528 (13)	0.0382 (11)	−0.0085 (10)	0.0008 (9)	−0.0031 (9)

C20	0.0718 (17)	0.0540 (14)	0.0444 (13)	−0.0104 (12)	−0.0014 (11)	0.0088 (11)
C21	0.084 (2)	0.0484 (14)	0.0593 (15)	−0.0265 (13)	−0.0030 (14)	0.0088 (11)
C22	0.0693 (16)	0.0461 (12)	0.0543 (13)	−0.0284 (11)	−0.0051 (11)	0.0021 (10)
C23	0.0346 (10)	0.0445 (11)	0.0379 (10)	−0.0116 (8)	0.0028 (8)	−0.0042 (8)
C24	0.0331 (10)	0.0432 (10)	0.0381 (10)	−0.0110 (8)	0.0036 (7)	−0.0096 (8)
N1	0.0790 (15)	0.0489 (11)	0.0667 (13)	−0.0343 (11)	0.0047 (11)	−0.0123 (10)
N2	0.0296 (8)	0.0399 (8)	0.0410 (8)	−0.0190 (6)	−0.0035 (6)	−0.0045 (7)
N3	0.0392 (9)	0.0405 (9)	0.0397 (9)	−0.0149 (7)	−0.0012 (7)	−0.0045 (7)
N4	0.0452 (10)	0.0415 (9)	0.0411 (9)	−0.0204 (7)	−0.0015 (7)	−0.0007 (7)
O1	0.0977 (15)	0.0558 (11)	0.0590 (11)	−0.0246 (10)	−0.0054 (10)	−0.0177 (9)
O2	0.0774 (14)	0.0730 (13)	0.1171 (18)	−0.0472 (11)	0.0106 (12)	−0.0407 (12)
O3	0.0340 (7)	0.0420 (8)	0.0600 (9)	−0.0213 (6)	−0.0038 (6)	0.0048 (7)
O4	0.0297 (7)	0.0552 (9)	0.0463 (8)	−0.0215 (6)	−0.0070 (6)	−0.0004 (6)

Geometric parameters (Å, °)

Cd1—N2	2.3059 (16)	C11—H11	0.9300
Cd1—O3^{i}	2.3385 (14)	C12—O4	1.241 (2)
Cd1—N4	2.3649 (17)	C12—O3	1.259 (2)
Cd1—O2	2.420 (2)	C12—Cd1^{ii}	2.7149 (18)
Cd1—O1	2.450 (2)	C13—N3	1.323 (3)
Cd1—O4^{i}	2.4526 (14)	C13—C14	1.398 (3)
Cd1—N3	2.4836 (17)	C13—H13	0.9300
Cd1—C12^{i}	2.7149 (18)	C14—C15	1.360 (4)
C1—N1	1.333 (3)	C14—H14	0.9300
C1—C2	1.379 (3)	C15—C16	1.402 (4)
C1—H1	0.9300	C15—H15	0.9300
C2—C3	1.382 (3)	C16—C24	1.401 (3)
C2—C6	1.497 (3)	C16—C17	1.433 (3)
C3—C4	1.381 (4)	C17—C18	1.334 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.371 (4)	C18—C19	1.420 (4)
C4—H4	0.9300	C18—H18	0.9300
C5—N1	1.313 (3)	C19—C20	1.404 (4)
C5—H5	0.9300	C19—C23	1.410 (3)
C6—O2	1.240 (3)	C20—C21	1.350 (4)
C6—O1	1.252 (3)	C20—H20	0.9300
C7—N2	1.339 (2)	C21—C22	1.390 (3)
C7—C8	1.381 (2)	C21—H21	0.9300
C7—H7	0.9300	C22—N4	1.327 (3)
C8—C9	1.383 (3)	C22—H22	0.9300
C8—C12	1.502 (2)	C23—N4	1.351 (3)
C9—C10	1.384 (3)	C23—C24	1.444 (3)
C9—H9	0.9300	C24—N3	1.350 (3)
C10—C11	1.377 (3)	O3—Cd1^{ii}	2.3385 (14)
C10—H10	0.9300	O4—Cd1^{ii}	2.4526 (14)
C11—N2	1.336 (3)		

N2—Cd1—O3^{i}	140.89 (5)	N2—C11—H11	118.5
N2—Cd1—N4	120.13 (6)	C10—C11—H11	118.5
O3^{i}—Cd1—N4	91.96 (6)	O4—C12—O3	123.82 (17)
N2—Cd1—O2	94.99 (7)	O4—C12—C8	118.82 (17)
O3^{i}—Cd1—O2	87.60 (6)	O3—C12—C8	117.34 (16)
N4—Cd1—O2	118.14 (7)	O4—C12—Cd1^{ii}	64.55 (10)
N2—Cd1—O1	84.12 (6)	O3—C12—Cd1^{ii}	59.33 (9)
O3^{i}—Cd1—O1	126.26 (6)	C8—C12—Cd1^{ii}	174.77 (13)
N4—Cd1—O1	79.62 (6)	N3—C13—C14	122.7 (2)
O2—Cd1—O1	53.38 (7)	N3—C13—H13	118.6
N2—Cd1—O4^{i}	86.27 (5)	C14—C13—H13	118.6
O3^{i}—Cd1—O4^{i}	54.76 (5)	C15—C14—C13	119.1 (2)
N4—Cd1—O4^{i}	138.04 (5)	C15—C14—H14	120.5
O2—Cd1—O4^{i}	88.14 (6)	C13—C14—H14	120.5
O1—Cd1—O4^{i}	139.06 (6)	C14—C15—C16	119.8 (2)
N2—Cd1—N3	91.80 (6)	C14—C15—H15	120.1
O3^{i}—Cd1—N3	79.14 (6)	C16—C15—H15	120.1
N4—Cd1—N3	68.45 (6)	C24—C16—C15	117.3 (2)
O2—Cd1—N3	165.57 (6)	C24—C16—C17	119.6 (2)
O1—Cd1—N3	140.29 (6)	C15—C16—C17	123.1 (2)
O4^{i}—Cd1—N3	79.60 (5)	C18—C17—C16	121.4 (2)
N2—Cd1—C12^{i}	113.35 (6)	C18—C17—H17	119.3
O3^{i}—Cd1—C12^{i}	27.59 (5)	C16—C17—H17	119.3
N4—Cd1—C12^{i}	115.76 (6)	C17—C18—C19	121.0 (2)
O2—Cd1—C12^{i}	88.34 (6)	C17—C18—H18	119.5
O1—Cd1—C12^{i}	140.09 (6)	C19—C18—H18	119.5
O4^{i}—Cd1—C12^{i}	27.19 (5)	C20—C19—C23	117.3 (2)
N3—Cd1—C12^{i}	77.27 (5)	C20—C19—C18	123.0 (2)
N1—C1—C2	124.7 (2)	C23—C19—C18	119.7 (2)
N1—C1—H1	117.7	C21—C20—C19	119.9 (2)
C2—C1—H1	117.7	C21—C20—H20	120.0
C1—C2—C3	117.0 (2)	C19—C20—H20	120.0
C1—C2—C6	120.8 (2)	C20—C21—C22	119.2 (2)
C3—C2—C6	122.1 (2)	C20—C21—H21	120.4
C4—C3—C2	119.2 (2)	C22—C21—H21	120.4
C4—C3—H3	120.4	N4—C22—C21	123.2 (2)
C2—C3—H3	120.4	N4—C22—H22	118.4
C5—C4—C3	118.2 (2)	C21—C22—H22	118.4
C5—C4—H4	120.9	N4—C23—C19	122.3 (2)
C3—C4—H4	120.9	N4—C23—C24	118.41 (18)
N1—C5—C4	124.3 (2)	C19—C23—C24	119.3 (2)
N1—C5—H5	117.8	N3—C24—C16	122.73 (19)
C4—C5—H5	117.8	N3—C24—C23	118.36 (18)
O2—C6—O1	122.7 (2)	C16—C24—C23	118.91 (19)
O2—C6—C2	119.7 (2)	C5—N1—C1	116.5 (2)

O1—C6—C2	117.6 (2)	C11—N2—C7	117.95 (16)
N2—C7—C8	123.01 (17)	C11—N2—Cd1	122.72 (12)
N2—C7—H7	118.5	C7—N2—Cd1	119.30 (12)
C8—C7—H7	118.5	C13—N3—C24	118.38 (19)
C7—C8—C9	118.31 (16)	C13—N3—Cd1	126.33 (15)
C7—C8—C12	119.94 (16)	C24—N3—Cd1	113.25 (13)
C9—C8—C12	121.74 (16)	C22—N4—C23	118.06 (19)
C8—C9—C10	119.18 (18)	C22—N4—Cd1	123.29 (16)
C8—C9—H9	120.4	C23—N4—Cd1	117.31 (13)
C10—C9—H9	120.4	C6—O1—Cd1	91.02 (16)
C11—C10—C9	118.61 (18)	C6—O2—Cd1	92.73 (17)
C11—C10—H10	120.7	C12—O3—Cd1^{ii}	93.08 (11)
C9—C10—H10	120.7	C12—O4—Cd1^{ii}	88.26 (11)
N2—C11—C10	122.92 (17)		

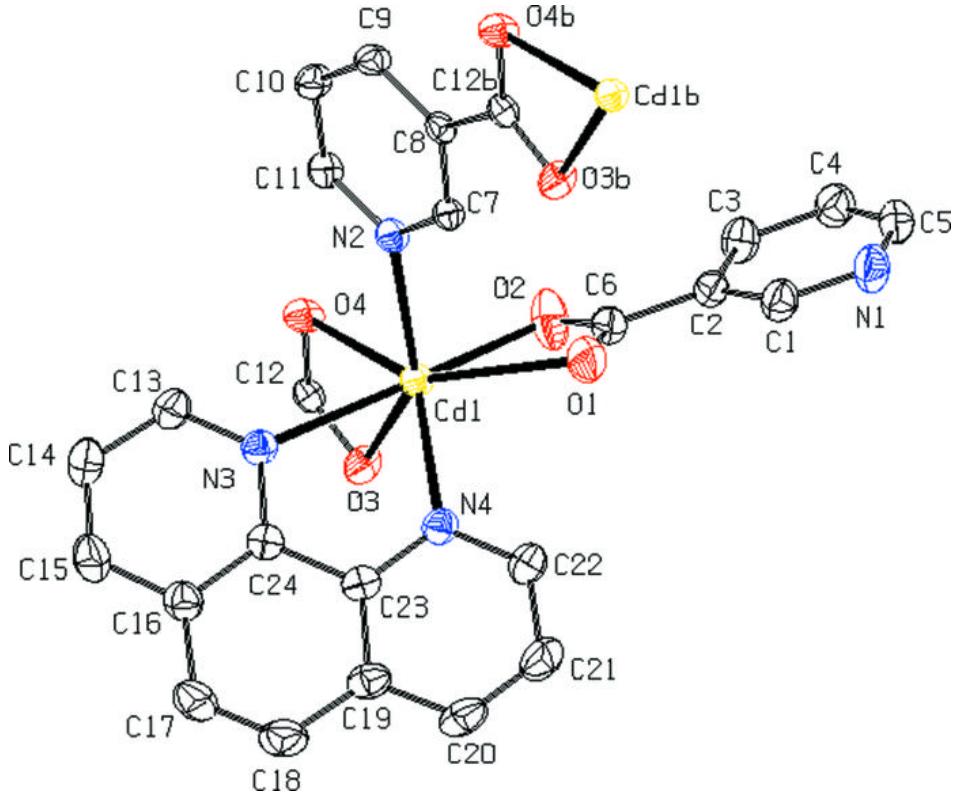
Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···Cg1^{iii}	0.93	2.97	3.853 (2)	158
C17—H17···Cg1^{iv}	0.93	2.67	3.435 (2)	140

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

Fig. 1


C9
O4b
C10
C12b
Cd1b
C8
C11
O3b
C4
C3
C7
C5
N2
O2
C6
O4
C2
N1
C1
C12
C13
Cd1
O1
C14
N3
O3
N4
C15
C24
C22
C23
C16
C21
C17
C19
C20
C18