Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[2,2′-Bis(pyridin-2-ylmethoxy)biphenyl-κ^4N,O,O',N']bis(nitrato-κ^2O,O')-cadmium

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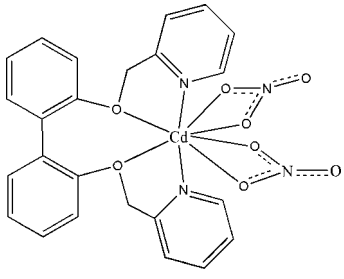
Received 28 August 2011; accepted 27 September 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.025; wR factor = 0.065; data-to-parameter ratio = 12.6.

In the title compound, $[Cd(NO_3)_2(C_{24}H_{20}N_2O_2)]$, the Cd^{II} ion is eight-coordinated by one ligand and two nitrate ions. There are C—H···O hydrogen bonds and C—H···π interactions and π–π interactions [centroid–centroid distance = 3.319 (1) Å] in the crystal structure.

Related literature

For background to weak intermolecular interactions, see: Desiraju & Steiner (2001); Reinhoudt & Crego-Calama (2002); Frederik & Mikkel (2001). For the synthesis of the 2,2′-bis(pyridin-2-ylmethoxy)biphenol ligand, see: Oh *et al.* (2005). For C—H···O and C—H···π hydrogen bonds, see: Guo *et al.* (2005). For aromatic ring arrangements, see: Janiak (2000).



Experimental

Crystal data

$[Cd(NO_3)_2(C_{24}H_{20}N_2O_2)]$
M_r = 604.84
Triclinic, $P\overline{1}$
a = 9.2216 (14) Å
b = 10.1064 (16) Å
c = 14.335 (2) Å
α = 73.723 (2)°
β = 73.501 (2)°
γ = 75.199 (2)°
V = 1207.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 293 K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.793, T_{max} = 1.000
6126 measured reflections
4197 independent reflections
3714 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.065
S = 1.05
4197 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

*Cg*2 and *Cg*3 are the centroids of the N2/C20–C24 and C7–C12 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6*B*···C4	0.97	2.67	3.278 (4)	121
C11—H11···O7^{i}	0.93	2.46	3.119 (3)	128
C15—H15···O8^{ii}	0.93	2.54	3.286 (4)	137
C19—H19*B*···O4^{iii}	0.97	2.49	3.411 (4)	159
C1—H1···O5^{iv}	0.93	2.58	3.317 (4)	136
C23—H23···O3^{v}	0.93	2.64	3.330 (4)	131
C17—H17···*Cg*2^{iii}	0.93	2.90	3.736 (3)	137
C22—H22···*Cg*3^{vi}	0.93	2.90	3.693 (3)	144

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

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-NT* (Bruker, 1998); data reduction: *SAINT-NT*; 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); software used to prepare material for publication: *SHELXTL*.

This work was supported financially by the Natural Science Foundation of Shanxi Normal University (ZR1012) and the Research Fund for the Doctoral Program of Shanxi Normal University (No. 833114).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2323).

References

Bruker, (1998). *SMART-NT* and *SAINT-NT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. & Steiner, T. (2001). *The Weak Hydrogen Bond in Structural Chemistry and Biology*. Oxford University Press.
Frederik, C. K. & Mikkel, J. (2001). *J. Org. Chem.* **66**, 6169–6173.
Guo, W.-S., Guo, F., Xu, H.-N., Yuan, L., Wang, Z.-H. & Tong, J. (2005). *J. Mol. Struct.* **733**, 143–149.
Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
Oh, M., Stern, C. L. & Mirkin, C. A. (2005). *Inorg. Chem.* **44**, 2647–2653.
Reinhoudt, D. N. & Crego-Calama, M. (2002). *Science*, **295**, 2403–2407.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, m1487 [doi:10.1107/S1600536811039687]

[2,2′-Bis(pyridin-2-ylmethoxy)biphenyl-κ^4N,O,O',N']bis(nitrato-κ^2O,O')cadmium

Cai-Juan Zhao and Rui-Feng Zhang

S1. Comment

In the past few years, there has been increasing interest in the study of weak intermolecular interactions, because of their important roles played in the various fields of chemistry and biochemistry, such as crystal engineering, supramolecular chemistry, molecular recognition and self-assembly of molecules (Desiraju *et al.*, 2001). Utilization of supramolecular architecture *via* non-covalent interactions is a vigorous field involving in the creation of new functional materials and is a powerful tool for particular structure formations (Reinhoudt *et al.*, 2002). Within the field of supramolecular chemistry, the non-covalent linkage of *p*-electron donating molecules to a *p*-deficient acceptor moiety through hydrogen bond and/or cooperative aromatic interactions (Frederik *et al.*, 2001) has attracted much attention in recent years. Recently, we have synthesized a coordination compound, namely [Cd(L_1)(NO_3)$_2$], (L_1 = 2,2′-bis(pyridin-2-ylmethyl)biphenol), which is constructed through non-covalent interactions.

The title compound crystallizes in triclinic space group P-1. The asymmetrical unit of the unit cell contains one Cd(II) ion, one ligand L_1 and two nitrate ions, as shown in Fig. 1. Each Cd(II) ion is eight-coordinated with four oxygen atoms from the two coordinated nitrate ions, two nitrogen and two oxygen atoms from the ligand L_1. The compound is then constructed into three-dimensional supramolecular structure through hydrogen bonds and π-π interactions. There are two kinds of hydrogen bonds (as shown in Fig. 2), C—H···O (H···O 2.460 (5)–2.895 (0) Å, O···O 3.118 (9)–3.412 (0) Å) and C—H···π (H···C 2.895 (0) Å, C···C 3.843 (1) Å) respectively, which is in good agreement with values reported in literature (Guo *et al.*, 2005). Both face-to-face and edge-to-face aromatic rings arrangements exist in compound, as shown in Fig. 3. For the face-to-face arrangement, the dihedral angle is 0.186° and the centroid-centroid distance is 3.319 (1) Å, within the effective distance 3.3–3.8 Å (Janiak, 2000). As for the edge-to-face arrangement, the dihedral angle is 107.41° and H···cg′ 2.900 (1) Å, C···cg′ 3.693 (4) Å, C—H···cg′ 144.04°, where C—H is from pyridine ring, and cg′ is the centroid of the phenol ring.

S2. Experimental

The title compound was prepared by adding 5 ml methanol solution of cadmium nitrate (0.3 mmol) to 10 ml methanol solution of L_1 (Oh *et al.*, 2005). The mixture was stirred for half an hour and filtered. The filtrate was slowly evaporated at room temperature to yield colorless block crystals suitable for X-ray analysis. Analysis calculated for $C_{24}H_{20}CdN_4O_8$: C 47.62, H 3.31, N 9.26%; found: C 48.06, H 3.09, N 9.49%.

S3. Refinement

Hydrogen atoms were included in calculated positions and refined with fixed thermal parameters riding on their parent atoms with C—H distances in the range of 0.93–0.97 Å, U_{iso}(H) = 1.2U_{eq}(C).

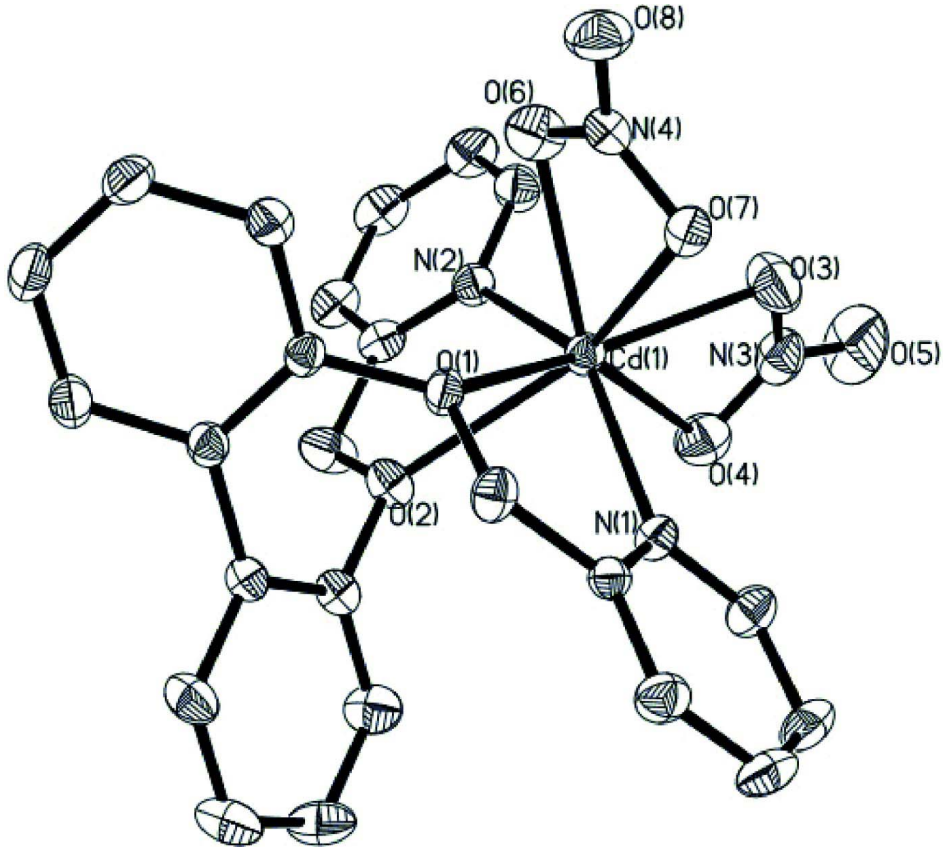


Figure 1

The thermal ellipsoid (30%) plot of coordination compound 1. Hydrogen atoms are omitted for clarity.

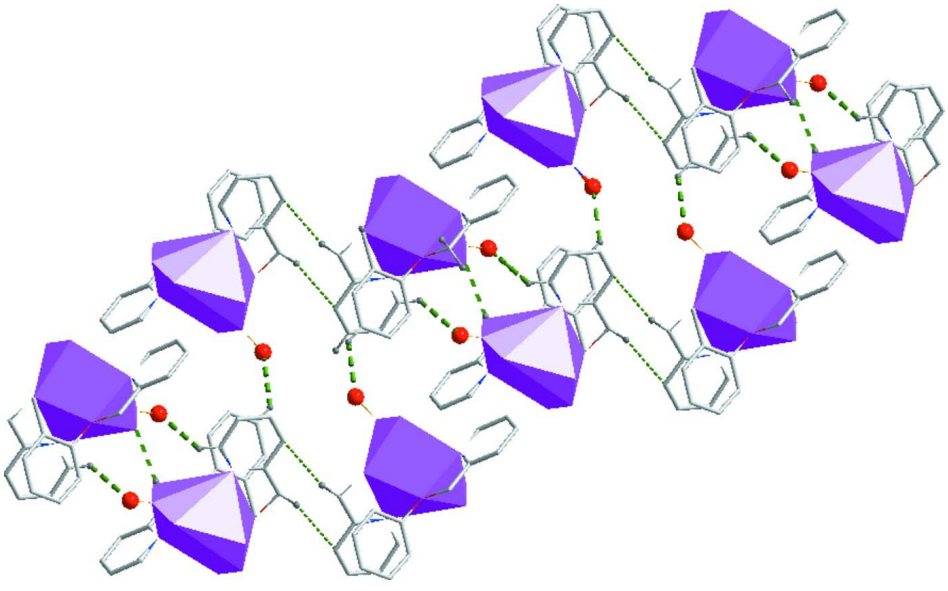


Figure 2

The hydrogen bonds of the title compound. Part of the hydrogen atoms are omitted for clarity.

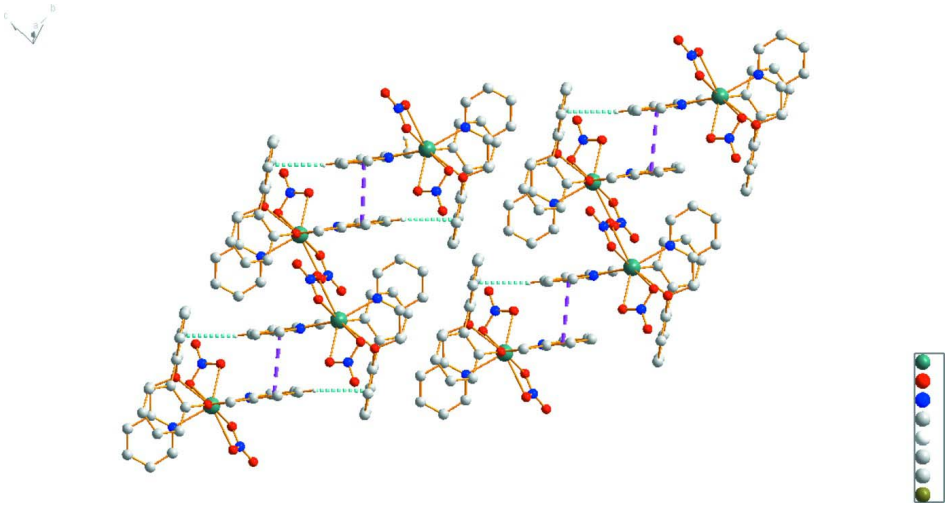


Figure 3

The π-π interactions of the title compound. Part of the hydrogen atoms are omitted for clarity.

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$b = 10.1064$ (16) Å
$c = 14.335$ (2) Å
$\alpha = 73.723$ (2)°
$\beta = 73.501$ (2)°
$\gamma = 75.199$ (2)°
$V = 1207.0$ (3) Å^3
$Z = 2$
$F(000) = 608$
$D_x = 1.664$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4044 reflections
$\theta = 2.4$–$26.3°$
$\mu = 0.96$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.793$, $T_{max} = 1.000$
6126 measured reflections
4197 independent reflections
3714 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 12$
$l = -17 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.065$
$S = 1.05$
4197 reflections
334 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
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.1926P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.81711 (2)	0.308586 (19)	0.326615 (13)	0.03353 (8)
O1	0.74199 (19)	0.35604 (18)	0.16450 (12)	0.0339 (4)
O2	0.5313 (2)	0.4063 (2)	0.34234 (12)	0.0410 (4)
O3	1.0172 (3)	0.2506 (3)	0.41079 (19)	0.0707 (7)
O4	0.8298 (3)	0.3957 (2)	0.47524 (16)	0.0622 (6)
O5	1.0254 (4)	0.3066 (4)	0.5432 (2)	0.1063 (11)
O6	0.8992 (2)	0.0848 (2)	0.27615 (15)	0.0565 (5)
O7	1.0435 (2)	0.2359 (2)	0.19232 (17)	0.0553 (5)
O8	1.0681 (3)	0.0488 (2)	0.14034 (17)	0.0594 (6)
N1	0.8489 (2)	0.5283 (2)	0.23165 (15)	0.0350 (5)
N2	0.6624 (2)	0.1800 (2)	0.45773 (15)	0.0380 (5)
N3	0.9588 (4)	0.3176 (3)	0.4785 (2)	0.0583 (7)
N4	1.0062 (3)	0.1209 (2)	0.20242 (18)	0.0426 (6)
C1	0.8922 (3)	0.6165 (3)	0.2697 (2)	0.0460 (7)
H1	0.9034	0.5875	0.3353	0.055*
C2	0.9203 (4)	0.7463 (3)	0.2163 (2)	0.0530 (8)
H2	0.9484	0.8047	0.2453	0.064*
C3	0.9061 (4)	0.7883 (3)	0.1194 (2)	0.0532 (8)
H3	0.9267	0.8752	0.0810	0.064*
C4	0.8610 (3)	0.7004 (3)	0.0791 (2)	0.0441 (7)
H4	0.8495	0.7280	0.0136	0.053*
C5	0.8331 (3)	0.5713 (2)	0.13708 (17)	0.0303 (5)
C6	0.7855 (3)	0.4773 (3)	0.09140 (18)	0.0374 (6)
H6A	0.6994	0.5291	0.0617	0.045*
H6B	0.8703	0.4477	0.0388	0.045*
C7	0.6315 (3)	0.2988 (3)	0.14698 (17)	0.0295 (5)
C8	0.6794 (3)	0.1738 (3)	0.11518 (19)	0.0371 (6)
H8	0.7830	0.1312	0.1035	0.044*
C9	0.5704 (3)	0.1131 (3)	0.1011 (2)	0.0438 (7)
H9	0.6005	0.0292	0.0798	0.053*
C10	0.4169 (3)	0.1775 (3)	0.1188 (2)	0.0458 (7)
H10	0.3439	0.1362	0.1101	0.055*
C11	0.3717 (3)	0.3021 (3)	0.1490 (2)	0.0417 (6)
H11	0.2682	0.3451	0.1593	0.050*
C12	0.4783 (3)	0.3659 (3)	0.16473 (18)	0.0327 (5)

C13	0.4303 (3)	0.5031 (3)	0.19484 (18)	0.0342 (6)
C14	0.3582 (3)	0.6212 (3)	0.1351 (2)	0.0462 (7)
H14	0.3376	0.6124	0.0775	0.055*
C15	0.3169 (4)	0.7502 (3)	0.1589 (2)	0.0572 (8)
H15	0.2674	0.8269	0.1184	0.069*
C16	0.3488 (4)	0.7660 (3)	0.2427 (2)	0.0600 (9)
H16	0.3225	0.8537	0.2582	0.072*
C17	0.4200 (4)	0.6515 (3)	0.3039 (2)	0.0520 (8)
H17	0.4408	0.6616	0.3610	0.062*
C18	0.4598 (3)	0.5223 (3)	0.27970 (18)	0.0364 (6)
C19	0.4273 (3)	0.3428 (3)	0.4250 (2)	0.0556 (8)
H19A	0.3531	0.3146	0.4019	0.067*
H19B	0.3715	0.4102	0.4656	0.067*
C20	0.5102 (3)	0.2170 (3)	0.48684 (19)	0.0396 (6)
C21	0.4245 (4)	0.1425 (3)	0.5720 (2)	0.0484 (7)
H21	0.3181	0.1703	0.5904	0.058*
C22	0.5004 (4)	0.0263 (3)	0.6289 (2)	0.0558 (8)
H22	0.4457	−0.0255	0.6864	0.067*
C23	0.6574 (4)	−0.0124 (3)	0.5998 (2)	0.0559 (8)
H23	0.7106	−0.0901	0.6375	0.067*
C24	0.7342 (4)	0.0652 (3)	0.5147 (2)	0.0483 (7)
H24	0.8405	0.0381	0.4950	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03440 (12)	0.03312 (12)	0.03341 (12)	−0.00985 (8)	−0.00953 (8)	−0.00311 (8)
O1	0.0330 (9)	0.0346 (10)	0.0375 (10)	−0.0129 (8)	−0.0124 (7)	−0.0031 (8)
O2	0.0371 (10)	0.0485 (11)	0.0298 (9)	−0.0054 (8)	−0.0068 (8)	−0.0004 (8)
O3	0.0536 (14)	0.0862 (19)	0.0803 (17)	0.0044 (13)	−0.0283 (12)	−0.0340 (15)
O4	0.0686 (16)	0.0581 (14)	0.0603 (14)	−0.0142 (12)	−0.0097 (12)	−0.0170 (11)
O5	0.140 (3)	0.130 (3)	0.084 (2)	−0.043 (2)	−0.077 (2)	−0.0106 (18)
O6	0.0565 (13)	0.0527 (13)	0.0484 (12)	−0.0115 (10)	−0.0015 (10)	−0.0021 (10)
O7	0.0378 (11)	0.0477 (13)	0.0888 (16)	−0.0089 (9)	−0.0126 (10)	−0.0299 (11)
O8	0.0602 (14)	0.0467 (13)	0.0676 (14)	−0.0026 (10)	−0.0014 (11)	−0.0276 (11)
N1	0.0371 (12)	0.0332 (12)	0.0362 (12)	−0.0126 (9)	−0.0071 (9)	−0.0059 (9)
N2	0.0389 (13)	0.0362 (12)	0.0375 (12)	−0.0099 (10)	−0.0086 (10)	−0.0036 (10)
N3	0.070 (2)	0.0621 (18)	0.0519 (16)	−0.0240 (15)	−0.0273 (14)	−0.0038 (14)
N4	0.0340 (13)	0.0391 (14)	0.0552 (15)	−0.0001 (10)	−0.0154 (11)	−0.0122 (12)
C1	0.0556 (18)	0.0448 (17)	0.0446 (16)	−0.0167 (14)	−0.0133 (13)	−0.0126 (13)
C2	0.063 (2)	0.0402 (17)	0.064 (2)	−0.0217 (15)	−0.0096 (16)	−0.0191 (15)
C3	0.067 (2)	0.0307 (16)	0.060 (2)	−0.0194 (14)	−0.0097 (16)	−0.0023 (14)
C4	0.0483 (17)	0.0377 (16)	0.0425 (16)	−0.0106 (13)	−0.0087 (13)	−0.0026 (12)
C5	0.0261 (12)	0.0291 (13)	0.0325 (13)	−0.0054 (10)	−0.0027 (10)	−0.0058 (10)
C6	0.0378 (15)	0.0442 (16)	0.0306 (13)	−0.0171 (12)	−0.0050 (11)	−0.0038 (11)
C7	0.0332 (13)	0.0299 (13)	0.0278 (13)	−0.0101 (10)	−0.0100 (10)	−0.0036 (10)
C8	0.0358 (14)	0.0370 (15)	0.0383 (15)	−0.0048 (12)	−0.0111 (11)	−0.0077 (12)
C9	0.0568 (19)	0.0344 (15)	0.0475 (17)	−0.0107 (13)	−0.0202 (14)	−0.0103 (12)

C10	0.0505 (18)	0.0474 (17)	0.0498 (17)	−0.0223 (14)	−0.0206 (14)	−0.0064 (14)
C11	0.0369 (15)	0.0463 (17)	0.0456 (16)	−0.0109 (12)	−0.0163 (12)	−0.0064 (13)
C12	0.0342 (14)	0.0339 (14)	0.0310 (13)	−0.0074 (11)	−0.0117 (10)	−0.0039 (10)
C13	0.0300 (13)	0.0358 (14)	0.0357 (14)	−0.0041 (11)	−0.0077 (11)	−0.0083 (11)
C14	0.0464 (17)	0.0492 (18)	0.0416 (16)	0.0049 (14)	−0.0190 (13)	−0.0116 (13)
C15	0.067 (2)	0.0442 (18)	0.0501 (19)	0.0137 (15)	−0.0201 (16)	−0.0095 (14)
C16	0.080 (2)	0.0361 (17)	0.058 (2)	0.0022 (16)	−0.0112 (17)	−0.0180 (15)
C17	0.068 (2)	0.0483 (18)	0.0407 (16)	−0.0039 (15)	−0.0151 (14)	−0.0162 (14)
C18	0.0333 (14)	0.0407 (15)	0.0323 (14)	−0.0045 (11)	−0.0071 (11)	−0.0063 (11)
C19	0.0441 (17)	0.0459 (18)	0.0545 (19)	−0.0027 (14)	0.0040 (14)	0.0030 (14)
C20	0.0494 (17)	0.0372 (15)	0.0316 (14)	−0.0114 (13)	−0.0048 (12)	−0.0085 (11)
C21	0.0533 (18)	0.0525 (18)	0.0381 (16)	−0.0193 (15)	0.0021 (13)	−0.0126 (14)
C22	0.083 (2)	0.0518 (19)	0.0320 (16)	−0.0274 (17)	−0.0073 (15)	−0.0001 (13)
C23	0.080 (2)	0.0466 (18)	0.0416 (17)	−0.0201 (17)	−0.0256 (16)	0.0081 (14)
C24	0.0497 (17)	0.0452 (17)	0.0478 (17)	−0.0114 (14)	−0.0185 (14)	0.0025 (14)

Geometric parameters (Å, º)

Cd1—N1	2.298 (2)	C7—C8	1.386 (3)
Cd1—N2	2.305 (2)	C7—C12	1.387 (3)
Cd1—O3	2.349 (2)	C8—C9	1.388 (4)
Cd1—O6	2.438 (2)	C8—H8	0.9300
Cd1—O1	2.4960 (16)	C9—C10	1.381 (4)
Cd1—O7	2.516 (2)	C9—H9	0.9300
Cd1—O2	2.5355 (18)	C10—C11	1.372 (4)
Cd1—O4	2.564 (2)	C10—H10	0.9300
O1—C7	1.402 (3)	C11—C12	1.402 (4)
O1—C6	1.433 (3)	C11—H11	0.9300
O2—C18	1.403 (3)	C12—C13	1.490 (4)
O2—C19	1.406 (3)	C13—C18	1.392 (4)
O3—N3	1.256 (3)	C13—C14	1.395 (4)
O4—N3	1.254 (3)	C14—C15	1.372 (4)
O5—N3	1.216 (3)	C14—H14	0.9300
O6—N4	1.265 (3)	C15—C16	1.373 (4)
O7—N4	1.253 (3)	C15—H15	0.9300
O8—N4	1.229 (3)	C16—C17	1.382 (4)
N1—C5	1.341 (3)	C16—H16	0.9300
N1—C1	1.353 (3)	C17—C18	1.377 (4)
N2—C20	1.331 (3)	C17—H17	0.9300
N2—C24	1.354 (3)	C19—C20	1.498 (4)
C1—C2	1.369 (4)	C19—H19A	0.9700
C1—H1	0.9300	C19—H19B	0.9700
C2—C3	1.368 (4)	C20—C21	1.387 (4)
C2—H2	0.9300	C21—C22	1.379 (4)
C3—C4	1.383 (4)	C21—H21	0.9300
C3—H3	0.9300	C22—C23	1.372 (5)
C4—C5	1.379 (4)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.364 (4)

C5—C6	1.500 (3)	C23—H23	0.9300
C6—H6A	0.9700	C24—H24	0.9300
C6—H6B	0.9700		

N1—Cd1—N2	146.09 (8)	C4—C5—C6	118.2 (2)
N1—Cd1—O3	101.09 (9)	O1—C6—C5	111.3 (2)
N2—Cd1—O3	92.68 (9)	O1—C6—H6A	109.4
N1—Cd1—O6	128.60 (7)	C5—C6—H6A	109.4
N2—Cd1—O6	81.38 (7)	O1—C6—H6B	109.4
O3—Cd1—O6	90.97 (8)	C5—C6—H6B	109.4
N1—Cd1—O1	68.38 (6)	H6A—C6—H6B	108.0
N2—Cd1—O1	113.32 (7)	C8—C7—C12	122.3 (2)
O3—Cd1—O1	147.49 (7)	C8—C7—O1	118.4 (2)
O6—Cd1—O1	74.91 (6)	C12—C7—O1	119.4 (2)
N1—Cd1—O7	81.60 (7)	C7—C8—C9	119.0 (2)
N2—Cd1—O7	131.70 (7)	C7—C8—H8	120.5
O3—Cd1—O7	79.53 (8)	C9—C8—H8	120.5
O6—Cd1—O7	51.57 (7)	C10—C9—C8	119.9 (3)
O1—Cd1—O7	68.70 (6)	C10—C9—H9	120.1
N1—Cd1—O2	85.15 (7)	C8—C9—H9	120.1
N2—Cd1—O2	66.24 (7)	C11—C10—C9	120.4 (3)
O3—Cd1—O2	143.64 (7)	C11—C10—H10	119.8
O6—Cd1—O2	113.14 (7)	C9—C10—H10	119.8
O1—Cd1—O2	68.10 (5)	C10—C11—C12	121.3 (3)
O7—Cd1—O2	136.72 (6)	C10—C11—H11	119.3
N1—Cd1—O4	86.65 (7)	C12—C11—H11	119.3
N2—Cd1—O4	78.09 (7)	C7—C12—C11	117.1 (2)
O3—Cd1—O4	51.22 (8)	C7—C12—C13	121.3 (2)
O6—Cd1—O4	135.23 (7)	C11—C12—C13	121.5 (2)
O1—Cd1—O4	149.86 (7)	C18—C13—C14	116.9 (2)
O7—Cd1—O4	125.77 (7)	C18—C13—C12	122.8 (2)
O2—Cd1—O4	94.10 (7)	C14—C13—C12	120.2 (2)
C7—O1—C6	115.83 (18)	C15—C14—C13	121.8 (3)
C7—O1—Cd1	125.97 (13)	C15—C14—H14	119.1
C6—O1—Cd1	116.20 (14)	C13—C14—H14	119.1
C18—O2—C19	113.6 (2)	C14—C15—C16	120.0 (3)
C18—O2—Cd1	128.07 (15)	C14—C15—H15	120.0
C19—O2—Cd1	118.32 (16)	C16—C15—H15	120.0
N3—O3—Cd1	101.28 (18)	C15—C16—C17	120.0 (3)
N3—O4—Cd1	90.90 (17)	C15—C16—H16	120.0
N4—O6—Cd1	96.57 (16)	C17—C16—H16	120.0
N4—O7—Cd1	93.15 (16)	C18—C17—C16	119.6 (3)
C5—N1—C1	117.9 (2)	C18—C17—H17	120.2
C5—N1—Cd1	122.44 (16)	C16—C17—H17	120.2
C1—N1—Cd1	119.62 (18)	C17—C18—C13	121.8 (2)
C20—N2—C24	117.8 (2)	C17—C18—O2	119.3 (2)
C20—N2—Cd1	124.93 (18)	C13—C18—O2	118.9 (2)
C24—N2—Cd1	116.98 (18)	O2—C19—C20	110.9 (2)

O5—N3—O4	122.5 (3)	O2—C19—H19A	109.5
O5—N3—O3	121.1 (3)	C20—C19—H19A	109.5
O4—N3—O3	116.4 (3)	O2—C19—H19B	109.5
O8—N4—O7	120.7 (2)	C20—C19—H19B	109.5
O8—N4—O6	121.5 (2)	H19A—C19—H19B	108.0
O7—N4—O6	117.8 (2)	N2—C20—C21	122.5 (3)
N1—C1—C2	123.1 (3)	N2—C20—C19	119.1 (2)
N1—C1—H1	118.5	C21—C20—C19	118.4 (3)
C2—C1—H1	118.5	C22—C21—C20	118.6 (3)
C3—C2—C1	118.5 (3)	C22—C21—H21	120.7
C3—C2—H2	120.7	C20—C21—H21	120.7
C1—C2—H2	120.7	C23—C22—C21	119.4 (3)
C2—C3—C4	119.4 (3)	C23—C22—H22	120.3
C2—C3—H3	120.3	C21—C22—H22	120.3
C4—C3—H3	120.3	C24—C23—C22	118.9 (3)
C5—C4—C3	119.2 (3)	C24—C23—H23	120.6
C5—C4—H4	120.4	C22—C23—H23	120.6
C3—C4—H4	120.4	N2—C24—C23	122.9 (3)
N1—C5—C4	121.9 (2)	N2—C24—H24	118.5
N1—C5—C6	119.9 (2)	C23—C24—H24	118.5

N1—Cd1—O1—C7	−151.15 (19)	O3—Cd1—N2—C24	−30.7 (2)
N2—Cd1—O1—C7	−7.90 (19)	O6—Cd1—N2—C24	59.9 (2)
O3—Cd1—O1—C7	132.55 (19)	O1—Cd1—N2—C24	129.28 (19)
O6—Cd1—O1—C7	65.53 (18)	O7—Cd1—N2—C24	47.7 (2)
O7—Cd1—O1—C7	119.66 (18)	O2—Cd1—N2—C24	180.0 (2)
O2—Cd1—O1—C7	−57.64 (17)	O4—Cd1—N2—C24	−80.1 (2)
O4—Cd1—O1—C7	−115.03 (19)	Cd1—O4—N3—O5	−175.6 (3)
N1—Cd1—O1—C6	12.00 (16)	Cd1—O4—N3—O3	4.6 (3)
N2—Cd1—O1—C6	155.25 (16)	Cd1—O3—N3—O5	175.1 (3)
O3—Cd1—O1—C6	−64.3 (2)	Cd1—O3—N3—O4	−5.1 (3)
O6—Cd1—O1—C6	−131.32 (17)	Cd1—O7—N4—O8	167.7 (2)
O7—Cd1—O1—C6	−77.19 (16)	Cd1—O7—N4—O6	−9.6 (2)
O2—Cd1—O1—C6	105.51 (17)	Cd1—O6—N4—O8	−167.3 (2)
O4—Cd1—O1—C6	48.1 (2)	Cd1—O6—N4—O7	9.9 (2)
N1—Cd1—O2—C18	21.51 (19)	C5—N1—C1—C2	0.0 (4)
N2—Cd1—O2—C18	−177.1 (2)	Cd1—N1—C1—C2	176.9 (2)
O3—Cd1—O2—C18	123.6 (2)	N1—C1—C2—C3	−1.0 (5)
O6—Cd1—O2—C18	−108.6 (2)	C1—C2—C3—C4	1.4 (5)
O1—Cd1—O2—C18	−47.12 (19)	C2—C3—C4—C5	−0.9 (5)
O7—Cd1—O2—C18	−50.8 (2)	C1—N1—C5—C4	0.6 (4)
O4—Cd1—O2—C18	107.8 (2)	Cd1—N1—C5—C4	−176.28 (19)
N1—Cd1—O2—C19	−155.9 (2)	C1—N1—C5—C6	179.9 (2)
N2—Cd1—O2—C19	5.5 (2)	Cd1—N1—C5—C6	3.1 (3)
O3—Cd1—O2—C19	−53.8 (3)	C3—C4—C5—N1	−0.1 (4)
O6—Cd1—O2—C19	74.0 (2)	C3—C4—C5—C6	−179.5 (3)
O1—Cd1—O2—C19	135.5 (2)	C7—O1—C6—C5	150.6 (2)
O7—Cd1—O2—C19	131.8 (2)	Cd1—O1—C6—C5	−14.3 (3)

O4—Cd1—O2—C19	−69.6 (2)	N1—C5—C6—O1	8.1 (3)
N1—Cd1—O3—N3	79.4 (2)	C4—C5—C6—O1	−172.5 (2)
N2—Cd1—O3—N3	−69.5 (2)	C6—O1—C7—C8	106.3 (2)
O6—Cd1—O3—N3	−150.9 (2)	Cd1—O1—C7—C8	−90.5 (2)
O1—Cd1—O3—N3	146.34 (17)	C6—O1—C7—C12	−75.6 (3)
O7—Cd1—O3—N3	158.5 (2)	Cd1—O1—C7—C12	87.6 (2)
O2—Cd1—O3—N3	−17.6 (3)	C12—C7—C8—C9	−0.4 (4)
O4—Cd1—O3—N3	2.88 (17)	O1—C7—C8—C9	177.6 (2)
N1—Cd1—O4—N3	−109.93 (18)	C7—C8—C9—C10	0.0 (4)
N2—Cd1—O4—N3	100.52 (18)	C8—C9—C10—C11	0.8 (4)
O3—Cd1—O4—N3	−2.83 (17)	C9—C10—C11—C12	−1.3 (4)
O6—Cd1—O4—N3	36.0 (2)	C8—C7—C12—C11	−0.1 (4)
O1—Cd1—O4—N3	−143.23 (16)	O1—C7—C12—C11	−178.1 (2)
O7—Cd1—O4—N3	−32.8 (2)	C8—C7—C12—C13	−177.5 (2)
O2—Cd1—O4—N3	165.18 (17)	O1—C7—C12—C13	4.6 (3)
N1—Cd1—O6—N4	23.7 (2)	C10—C11—C12—C7	0.9 (4)
N2—Cd1—O6—N4	−173.92 (17)	C10—C11—C12—C13	178.3 (2)
O3—Cd1—O6—N4	−81.35 (16)	C7—C12—C13—C18	−58.0 (4)
O1—Cd1—O6—N4	68.99 (15)	C11—C12—C13—C18	124.7 (3)
O7—Cd1—O6—N4	−5.57 (14)	C7—C12—C13—C14	119.2 (3)
O2—Cd1—O6—N4	126.62 (15)	C11—C12—C13—C14	−58.0 (4)
O4—Cd1—O6—N4	−110.62 (16)	C18—C13—C14—C15	−0.5 (4)
N1—Cd1—O7—N4	−151.69 (16)	C12—C13—C14—C15	−177.9 (3)
N2—Cd1—O7—N4	21.10 (19)	C13—C14—C15—C16	1.1 (5)
O3—Cd1—O7—N4	105.31 (17)	C14—C15—C16—C17	−1.1 (5)
O6—Cd1—O7—N4	5.59 (14)	C15—C16—C17—C18	0.6 (5)
O1—Cd1—O7—N4	−81.70 (15)	C16—C17—C18—C13	0.0 (5)
O2—Cd1—O7—N4	−78.05 (18)	C16—C17—C18—O2	−179.7 (3)
O4—Cd1—O7—N4	128.63 (15)	C14—C13—C18—C17	0.0 (4)
N2—Cd1—N1—C5	−107.9 (2)	C12—C13—C18—C17	177.3 (3)
O3—Cd1—N1—C5	139.97 (19)	C14—C13—C18—O2	179.6 (2)
O6—Cd1—N1—C5	39.7 (2)	C12—C13—C18—O2	−3.0 (4)
O1—Cd1—N1—C5	−7.88 (17)	C19—O2—C18—C17	82.6 (3)
O7—Cd1—N1—C5	62.46 (19)	Cd1—O2—C18—C17	−94.9 (3)
O2—Cd1—N1—C5	−76.23 (19)	C19—O2—C18—C13	−97.0 (3)
O4—Cd1—N1—C5	−170.63 (19)	Cd1—O2—C18—C13	85.4 (3)
N2—Cd1—N1—C1	75.3 (2)	C18—O2—C19—C20	178.1 (2)
O3—Cd1—N1—C1	−36.8 (2)	Cd1—O2—C19—C20	−4.2 (3)
O6—Cd1—N1—C1	−137.1 (2)	C24—N2—C20—C21	−0.3 (4)
O1—Cd1—N1—C1	175.3 (2)	Cd1—N2—C20—C21	−173.7 (2)
O7—Cd1—N1—C1	−114.3 (2)	C24—N2—C20—C19	−179.5 (3)
O2—Cd1—N1—C1	107.0 (2)	Cd1—N2—C20—C19	7.0 (4)
O4—Cd1—N1—C1	12.6 (2)	O2—C19—C20—N2	−1.2 (4)
N1—Cd1—N2—C20	28.3 (3)	O2—C19—C20—C21	179.5 (3)
O3—Cd1—N2—C20	142.8 (2)	N2—C20—C21—C22	0.5 (4)
O6—Cd1—N2—C20	−126.6 (2)	C19—C20—C21—C22	179.7 (3)
O1—Cd1—N2—C20	−57.2 (2)	C20—C21—C22—C23	−0.1 (5)
O7—Cd1—N2—C20	−138.85 (19)	C21—C22—C23—C24	−0.4 (5)

O2—Cd1—N2—C20	−6.54 (19)	C20—N2—C24—C23	−0.3 (4)
O4—Cd1—N2—C20	93.4 (2)	Cd1—N2—C24—C23	173.7 (2)
N1—Cd1—N2—C24	−145.19 (19)	C22—C23—C24—N2	0.6 (5)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the N2/C20–C24 and C7–C12 rings ,respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*B*···C4	0.97	2.67	3.278 (4)	121
C11—H11···O7^{i}	0.93	2.46	3.119 (3)	128
C15—H15···O8^{ii}	0.93	2.54	3.286 (4)	137
C19—H19*B*···O4^{iii}	0.97	2.49	3.411 (4)	159
C1—H1···O5^{iv}	0.93	2.58	3.317 (4)	136
C23—H23···O3^{v}	0.93	2.64	3.330 (4)	131
C17—H17···*Cg*2^{iii}	0.93	2.90	3.736 (3)	137
C22—H22···*Cg*3^{vi}	0.93	2.90	3.693 (3)	144

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