

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Bis[2-hydroxy-*N'*-(2-hydroxybenzoyl)-benzohydrazitato]dipyridinecadmium(II)

Yu-Ting Chen^{a,b} and Da-Cheng Li^{b*}

^aDepartment of Chemistry, Dezhou University, Dezhou 253023, People's Republic of China, and ^bCollege of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China

Correspondence e-mail: lidacheng@lcu.edu.cn

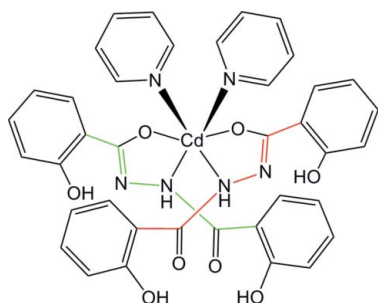
Received 8 August 2008; accepted 22 October 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.027; wR factor = 0.071; data-to-parameter ratio = 13.1.

The title complex, $[\text{Cd}(\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}_4)_2(\text{C}_5\text{H}_5\text{N})_2]$, exhibits crystallographic twofold symmetry. The Cd^{II} atom is located on the twofold rotation axis and reveals a slightly distorted octahedral coordination defined by four atoms (N_2O_2) from two symmetry-related chelate ligands and two pyridine N atoms. Intramolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds stabilize the molecular conformation while intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding links molecules into a triad, generating a helix along the threefold screw axis.

Related literature

Three manganese metallacrowns with unsymmetrical aroylhydrazine ligands were synthesized and reported by Dou *et al.* (2006) and John *et al.* (2006). For the crystal structure of an iron compound with *N,N'*-bis-picolinoyl hydrazine, see: Bernhardt *et al.* (2005). For a nickel complex formed by *N,N'*-disalicyloylhydrazine, see: Chen *et al.* (2007).



Experimental

Crystal data

$[\text{Cd}(\text{C}_{14}\text{H}_{11}\text{N}_2\text{O}_4)_2(\text{C}_5\text{H}_5\text{N})_2]$
 $M_r = 813.10$
 Trigonal, $P3_121$
 $a = 13.0380$ (10) Å

$c = 18.069$ (3) Å
 $V = 2660.0$ (5) Å³
 $Z = 3$
 Mo $K\alpha$ radiation

$\mu = 0.68$ mm⁻¹
 $T = 298$ (2) K

0.40 × 0.38 × 0.35 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.773$, $T_{\text{max}} = 0.797$

13955 measured reflections
 3146 independent reflections
 2750 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.071$
 $S = 1.00$
 3146 reflections
 241 parameters
 H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.90$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³
 Absolute structure: Flack (1983),
 1353 Friedel pairs
 Flack parameter: -0.06 (3)

Table 1

Selected bond lengths (Å).

Cd1—N1	2.331 (3)	Cd1—O1	2.389 (2)
Cd1—N3	2.337 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O4—H4 \cdots O3	0.82	1.92	2.638 (4)	145
N2—H2 \cdots O2	0.86	1.94	2.624 (4)	135
O2—H2A \cdots O3 ⁱ	0.82	1.88	2.639 (3)	153

Symmetry code: (i) $x - y, -y, -z + \frac{2}{3}$.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors acknowledge the support of the National Natural Science Foundation of China (grant No. 20671048).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2188).

References

- Bernhardt, P. V., Chin, P., Sharpe, P. C., Wang, J. C. & Richardson, D. R. (2005). *Biol. Inorg. Chem.* **10**, 761–777.
 Chen, Y.-T., Dou, J.-M., Li, D.-C., Wang, D.-Q. & Zhu, Y.-H. (2007). *Acta Cryst. E63*, m2503–m2504.
 Dou, J. M., Liu, M. L., Li, D. C. & Wang, D. Q. (2006). *Eur. J. Inorg. Chem.* **23**, 4866–4871.
 Flack, H. D. (1983). *Acta Cryst. A39*, 876–881.
 John, R. P., Park, J., Moon, D., Lee, K. & Lah, M. S. (2006). *Chem. Commun.* pp. 3699–3701.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst. A64*, 112–122.
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2008). E64, m1466 [doi:10.1107/S1600536808034533]

Bis[2-hydroxy-*N'*-(2-hydroxybenzoyl)benzohydrazitato]dipyridinecadmium(II)

Y.-T. Chen and D.-C. Li

Comment

Metal complexes with aroylhydrazine ligands are of increasing attention due to their interesting chemical activities (John *et al.* 2006; Dou *et al.*, 2006). However, the research on the compounds with symmetrical diaroylhydrazine ligands was limited (Bernhardt *et al.*, 2005; Chen *et al.*, 2007). As an extension of our work on the structural characterization of these compounds, the title complex, (I), is synthesized and characterized by X-ray structure analysis. The complex (I) exhibits a twofold rotation symmetry. It comprises of one Cd^{II} atom at special position at the twofold rotation axes coordinated by two ligands and two pyridines (Fig. 1 and Table 1). Each ligand acts as the bidentate via the iminoacyl groups forming two five-membered rings around metal ion with the dihedral angle of 59.71 (4)°.

Intramolecular O4—H4···O3 and N2—H2···O2 hydrogen bonds stabilizes the molecular conformation. There is also an intermolecular hydrogen bond O—H···O hydrogen bond [2.639 (3) Å] (Table 2) assembling three molecules into a triad, that is a basic structural element of a helix along [0 0 1] direction (Fig. 2).

Experimental

The solution of Cd(NO₃)₂·4H₂O (0.123 g, 0.4 mmol) in methanol (10 mL) was added to the mixture of 1,2-disalicyloylhydrazine (0.054 g, 0.2 mmol) and sodium hydroxide (0.032 g, 0.8 mmol) in pyridine (10 mL). A colourless solution was generated after stirring for two hours at room temperature. The solution was allowed to stand for 2 weeks, whereupon white block crystals were obtained. Yield: 0.058 g, 77%. m. p. > 573 K. Anal. for C₃₈H₃₂CdN₆O₈: Calc. C, 56.08; H, 3.93; N, 10.33; Found: C, 56.54; H, 3.71; N, 10.54%. The No. of CCDC: 686345.

Refinement

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms with C(*sp*₂ hybrid)-H distances of 0.93 Å (*U*_{iso}(H)=1.2*U*_{eq}(C)).

Figures

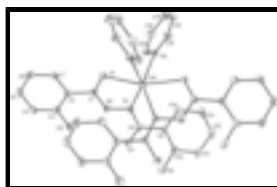


Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level.

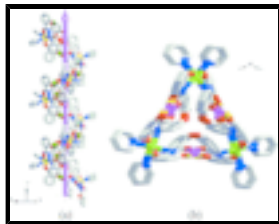


Fig. 2. Supramolecular structure of the title complex in the direction [001].

Bis[2-hydroxy-N'-(2-hydroxybenzoyl)benzohydrazitato]dipyridinecadmium(II)

Crystal data

[Cd(C₁₄H₁₁N₂O₄)₂(C₅H₅N)₂]

M_r = 813.10

Trigonal, *P*3₁21

a = 13.0380 (10) Å

b = 13.0380 (10) Å

c = 18.069 (3) Å

α = 90°

β = 90°

γ = 120°

V = 2660.0 (5) Å³

Z = 3

*F*₀₀₀ = 1242

D_x = 1.523 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 5141 reflections

θ = 2.9–22.9°

μ = 0.68 mm⁻¹

T = 298 (2) K

Block, colourless

0.40 × 0.38 × 0.35 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 298(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

*T*_{min} = 0.773, *T*_{max} = 0.797

13955 measured reflections

3146 independent reflections

2750 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.033

θ_{max} = 25.0°

θ_{min} = 1.8°

h = -15→15

k = -15→15

l = -21→10

Refinement

Refinement on *F*²

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

wR(*F*²) = 0.071

S = 1.00

3146 reflections

241 parameters

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.5675P]$

where $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)_{max} < 0.001

$\Delta\rho_{\text{max}} = 0.90 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$

Extinction correction: none

Primary atom site location: structure-invariant direct methods Absolute structure: Flack (1983), 1353 Friedel pairs
 Secondary atom site location: difference Fourier map Flack parameter: -0.06 (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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	1.0000	0.45722 (2)	0.6667	0.04088 (11)
N1	0.8620 (2)	0.2612 (2)	0.69499 (15)	0.0387 (7)
N2	0.8356 (3)	0.2467 (3)	0.77051 (14)	0.0406 (6)
H2	0.8005	0.1771	0.7897	0.049*
N3	0.8726 (2)	0.5186 (3)	0.61934 (16)	0.0449 (7)
O1	0.9119 (2)	0.4418 (2)	0.78506 (13)	0.0517 (7)
O2	0.7567 (3)	0.1137 (2)	0.88928 (14)	0.0584 (7)
H2A	0.7290	0.0561	0.9170	0.088*
O3	0.8013 (3)	0.06392 (19)	0.69676 (12)	0.0558 (6)
O4	0.9060 (3)	0.0079 (3)	0.59233 (16)	0.0797 (10)
H4	0.8760	0.0022	0.6331	0.120*
C1	0.8648 (3)	0.3405 (3)	0.81227 (18)	0.0391 (8)
C2	0.8409 (3)	0.3228 (3)	0.89327 (19)	0.0403 (8)
C3	0.7918 (3)	0.2136 (4)	0.9296 (2)	0.0454 (9)
C4	0.7786 (4)	0.2086 (4)	1.0058 (2)	0.0548 (10)
H4A	0.7467	0.1360	1.0298	0.066*
C5	0.8122 (4)	0.3102 (4)	1.0464 (2)	0.0614 (11)
H5	0.8012	0.3053	1.0974	0.074*
C6	0.8618 (4)	0.4184 (4)	1.0120 (2)	0.0556 (10)
H6	0.8858	0.4872	1.0393	0.067*
C7	0.8753 (3)	0.4233 (3)	0.9357 (2)	0.0477 (9)
H7	0.9085	0.4965	0.9123	0.057*
C8	0.8396 (3)	0.1621 (3)	0.66318 (18)	0.0402 (8)
C9	0.8647 (3)	0.1680 (3)	0.58281 (18)	0.0415 (8)
C10	0.9002 (4)	0.0938 (4)	0.5519 (2)	0.0547 (10)
C11	0.9321 (4)	0.1039 (4)	0.4769 (2)	0.0687 (13)
H11	0.9592	0.0562	0.4568	0.082*
C12	0.9225 (4)	0.1852 (4)	0.4338 (2)	0.0673 (12)
H12	0.9435	0.1926	0.3841	0.081*
C13	0.8832 (4)	0.2547 (4)	0.4624 (2)	0.0629 (12)

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H13	0.8754	0.3080	0.4320	0.075*
C14	0.8542 (3)	0.2472 (4)	0.5364 (2)	0.0516 (9)
H14	0.8274	0.2958	0.5555	0.062*
C15	0.9145 (4)	0.6185 (4)	0.5806 (2)	0.0550 (10)
H15	0.9942	0.6587	0.5675	0.066*
C16	0.8437 (4)	0.6645 (4)	0.5591 (2)	0.0636 (12)
H16	0.8760	0.7358	0.5334	0.076*
C17	0.7270 (4)	0.6045 (4)	0.5759 (2)	0.0627 (12)
H17	0.6777	0.6335	0.5616	0.075*
C18	0.6827 (3)	0.5002 (4)	0.6144 (2)	0.0591 (11)
H18	0.6026	0.4570	0.6263	0.071*
C19	0.7572 (3)	0.4610 (3)	0.6349 (2)	0.0535 (9)
H19	0.7262	0.3903	0.6612	0.064*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0445 (2)	0.03796 (14)	0.04239 (18)	0.02224 (11)	0.00869 (17)	0.00434 (9)
N1	0.0392 (17)	0.0368 (16)	0.0340 (15)	0.0144 (14)	0.0019 (12)	0.0033 (12)
N2	0.0437 (16)	0.0396 (16)	0.0347 (15)	0.0179 (13)	0.0072 (13)	0.0058 (14)
N3	0.0448 (18)	0.0430 (17)	0.0494 (17)	0.0236 (15)	0.0064 (13)	0.0045 (14)
O1	0.0692 (18)	0.0398 (14)	0.0459 (15)	0.0271 (13)	0.0147 (13)	0.0067 (12)
O2	0.080 (2)	0.0438 (15)	0.0434 (15)	0.0254 (14)	0.0077 (13)	0.0107 (13)
O3	0.0734 (19)	0.0376 (13)	0.0493 (14)	0.0223 (15)	0.0222 (15)	0.0080 (11)
O4	0.118 (3)	0.081 (2)	0.066 (2)	0.070 (2)	0.0278 (19)	0.0082 (17)
C1	0.0388 (19)	0.041 (2)	0.041 (2)	0.0226 (17)	0.0035 (16)	0.0036 (17)
C2	0.042 (2)	0.049 (2)	0.0364 (18)	0.0282 (17)	0.0029 (15)	0.0027 (16)
C3	0.044 (2)	0.056 (2)	0.042 (2)	0.0290 (18)	0.0009 (16)	0.0031 (18)
C4	0.065 (3)	0.066 (3)	0.042 (2)	0.040 (2)	0.0030 (19)	0.012 (2)
C5	0.074 (3)	0.092 (4)	0.037 (2)	0.055 (3)	0.005 (2)	0.006 (2)
C6	0.064 (3)	0.073 (3)	0.048 (2)	0.048 (2)	-0.0070 (19)	-0.011 (2)
C7	0.055 (2)	0.049 (2)	0.049 (2)	0.0344 (19)	0.0047 (17)	0.0020 (17)
C8	0.0341 (18)	0.0382 (17)	0.0420 (17)	0.0133 (15)	0.0033 (15)	0.0030 (14)
C9	0.038 (2)	0.0391 (17)	0.0363 (16)	0.0113 (17)	0.0027 (16)	-0.0017 (13)
C10	0.063 (3)	0.049 (2)	0.047 (2)	0.025 (2)	0.005 (2)	-0.0025 (18)
C11	0.077 (3)	0.076 (3)	0.046 (2)	0.033 (3)	0.011 (2)	-0.011 (2)
C12	0.065 (3)	0.073 (3)	0.039 (2)	0.016 (2)	0.004 (2)	-0.006 (2)
C13	0.065 (3)	0.061 (2)	0.040 (2)	0.014 (2)	-0.010 (2)	0.0026 (18)
C14	0.047 (2)	0.044 (2)	0.050 (2)	0.0129 (17)	-0.0035 (18)	-0.0011 (19)
C15	0.050 (2)	0.056 (2)	0.060 (3)	0.027 (2)	0.0090 (18)	0.012 (2)
C16	0.069 (3)	0.067 (3)	0.062 (2)	0.040 (2)	0.007 (2)	0.025 (2)
C17	0.065 (3)	0.088 (3)	0.053 (2)	0.051 (3)	-0.006 (2)	0.002 (2)
C18	0.041 (2)	0.074 (3)	0.062 (3)	0.028 (2)	-0.0012 (19)	-0.007 (2)
C19	0.048 (2)	0.044 (2)	0.063 (2)	0.0198 (19)	0.0099 (19)	0.0037 (19)

Geometric parameters (\AA , $^\circ$)

Cd1—N1	2.331 (3)	C5—H5	0.9300
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Cd1—N1 ⁱ	2.331 (3)	C6—C7	1.387 (5)
Cd1—N3 ⁱ	2.337 (3)	C6—H6	0.9300
Cd1—N3	2.337 (3)	C7—H7	0.9300
Cd1—O1	2.389 (2)	C8—C9	1.482 (4)
Cd1—O1 ⁱ	2.389 (2)	C9—C10	1.382 (5)
N1—C8	1.307 (4)	C9—C14	1.389 (5)
N1—N2	1.397 (4)	C10—C11	1.404 (5)
N2—C1	1.320 (4)	C11—C12	1.371 (6)
N2—H2	0.8600	C11—H11	0.9300
N3—C15	1.332 (5)	C12—C13	1.346 (6)
N3—C19	1.333 (5)	C12—H12	0.9300
O1—C1	1.245 (4)	C13—C14	1.380 (5)
O2—C3	1.357 (4)	C13—H13	0.9300
O2—H2A	0.8200	C14—H14	0.9300
O3—C8	1.271 (4)	C15—C16	1.385 (6)
O4—C10	1.371 (5)	C15—H15	0.9300
O4—H4	0.8200	C16—C17	1.352 (6)
C1—C2	1.490 (5)	C16—H16	0.9300
C2—C7	1.385 (5)	C17—C18	1.372 (6)
C2—C3	1.399 (5)	C17—H17	0.9300
C3—C4	1.384 (5)	C18—C19	1.356 (6)
C4—C5	1.380 (6)	C18—H18	0.9300
C4—H4A	0.9300	C19—H19	0.9300
C5—C6	1.372 (6)		
N1—Cd1—N1 ⁱ	89.45 (14)	C5—C6—C7	118.8 (4)
N1—Cd1—N3 ⁱ	145.80 (9)	C5—C6—H6	120.6
N1 ⁱ —Cd1—N3 ⁱ	99.48 (10)	C7—C6—H6	120.6
N1—Cd1—N3	99.48 (10)	C2—C7—C6	122.2 (4)
N1 ⁱ —Cd1—N3	145.80 (9)	C2—C7—H7	118.9
N3 ⁱ —Cd1—N3	91.48 (14)	C6—C7—H7	118.9
N1—Cd1—O1	68.64 (9)	O3—C8—N1	124.5 (3)
N1 ⁱ —Cd1—O1	125.88 (9)	O3—C8—C9	119.0 (3)
N3 ⁱ —Cd1—O1	79.62 (9)	N1—C8—C9	116.4 (3)
N3—Cd1—O1	87.84 (9)	C10—C9—C14	117.9 (3)
N1—Cd1—O1 ⁱ	125.88 (9)	C10—C9—C8	120.1 (3)
N1 ⁱ —Cd1—O1 ⁱ	68.64 (9)	C14—C9—C8	121.9 (3)
N3 ⁱ —Cd1—O1 ⁱ	87.84 (9)	O4—C10—C9	122.1 (3)
N3—Cd1—O1 ⁱ	79.62 (9)	O4—C10—C11	117.1 (4)
O1—Cd1—O1 ⁱ	162.04 (12)	C9—C10—C11	120.7 (4)
C8—N1—N2	112.2 (3)	C12—C11—C10	118.9 (4)
C8—N1—Cd1	131.0 (2)	C12—C11—H11	120.5
N2—N1—Cd1	111.44 (19)	C10—C11—H11	120.5
C1—N2—N1	119.7 (3)	C13—C12—C11	121.0 (4)
C1—N2—H2	120.1	C13—C12—H12	119.5
N1—N2—H2	120.1	C11—C12—H12	119.5
C15—N3—C19	117.2 (3)	C12—C13—C14	120.4 (4)

supplementary materials

C15—N3—Cd1	120.9 (2)	C12—C13—H13	119.8
C19—N3—Cd1	121.7 (2)	C14—C13—H13	119.8
C1—O1—Cd1	113.9 (2)	C13—C14—C9	120.9 (4)
C3—O2—H2A	109.5	C13—C14—H14	119.6
C10—O4—H4	109.5	C9—C14—H14	119.6
O1—C1—N2	121.1 (3)	N3—C15—C16	122.3 (4)
O1—C1—C2	120.4 (3)	N3—C15—H15	118.8
N2—C1—C2	118.5 (3)	C16—C15—H15	118.8
C7—C2—C3	118.0 (3)	C17—C16—C15	119.2 (4)
C7—C2—C1	117.0 (3)	C17—C16—H16	120.4
C3—C2—C1	124.9 (3)	C15—C16—H16	120.4
O2—C3—C4	121.0 (4)	C16—C17—C18	118.8 (4)
O2—C3—C2	119.2 (3)	C16—C17—H17	120.6
C4—C3—C2	119.8 (4)	C18—C17—H17	120.6
C5—C4—C3	120.8 (4)	C19—C18—C17	119.1 (4)
C5—C4—H4A	119.6	C19—C18—H18	120.5
C3—C4—H4A	119.6	C17—C18—H18	120.5
C6—C5—C4	120.4 (4)	N3—C19—C18	123.3 (4)
C6—C5—H5	119.8	N3—C19—H19	118.3
C4—C5—H5	119.8	C18—C19—H19	118.3
N1 ⁱ —Cd1—N1—C8	-39.3 (3)	C7—C2—C3—C4	0.2 (5)
N3 ⁱ —Cd1—N1—C8	-145.5 (3)	C1—C2—C3—C4	177.0 (4)
N3—Cd1—N1—C8	107.5 (3)	O2—C3—C4—C5	-178.7 (4)
O1—Cd1—N1—C8	-168.6 (3)	C2—C3—C4—C5	0.7 (6)
O1 ⁱ —Cd1—N1—C8	23.6 (3)	C3—C4—C5—C6	-1.4 (6)
N1 ⁱ —Cd1—N1—N2	112.3 (2)	C4—C5—C6—C7	1.2 (6)
N3 ⁱ —Cd1—N1—N2	6.1 (3)	C3—C2—C7—C6	-0.4 (5)
N3—Cd1—N1—N2	-100.9 (2)	C1—C2—C7—C6	-177.5 (3)
O1—Cd1—N1—N2	-17.02 (19)	C5—C6—C7—C2	-0.3 (6)
O1 ⁱ —Cd1—N1—N2	175.09 (18)	N2—N1—C8—O3	-1.8 (5)
C8—N1—N2—C1	172.8 (3)	Cd1—N1—C8—O3	149.6 (3)
Cd1—N1—N2—C1	15.7 (3)	N2—N1—C8—C9	180.0 (3)
N1—Cd1—N3—C15	-164.9 (3)	Cd1—N1—C8—C9	-28.6 (4)
N1 ⁱ —Cd1—N3—C15	-61.7 (4)	O3—C8—C9—C10	-30.0 (5)
N3 ⁱ —Cd1—N3—C15	47.6 (3)	N1—C8—C9—C10	148.3 (3)
O1—Cd1—N3—C15	127.1 (3)	O3—C8—C9—C14	150.3 (4)
O1 ⁱ —Cd1—N3—C15	-39.9 (3)	N1—C8—C9—C14	-31.4 (5)
N1—Cd1—N3—C19	20.6 (3)	C14—C9—C10—O4	-175.9 (4)
N1 ⁱ —Cd1—N3—C19	123.8 (3)	C8—C9—C10—O4	4.4 (6)
N3 ⁱ —Cd1—N3—C19	-126.9 (3)	C14—C9—C10—C11	4.1 (6)
O1—Cd1—N3—C19	-47.3 (3)	C8—C9—C10—C11	-175.6 (4)
O1 ⁱ —Cd1—N3—C19	145.6 (3)	O4—C10—C11—C12	177.2 (4)
N1—Cd1—O1—C1	19.5 (2)	C9—C10—C11—C12	-2.9 (7)
N1 ⁱ —Cd1—O1—C1	-53.3 (3)	C10—C11—C12—C13	-0.1 (7)
N3 ⁱ —Cd1—O1—C1	-147.5 (3)	C11—C12—C13—C14	1.6 (7)
N3—Cd1—O1—C1	120.5 (2)	C12—C13—C14—C9	-0.2 (6)

O1 ⁱ —Cd1—O1—C1	166.0 (2)	C10—C9—C14—C13	-2.6 (5)
Cd1—O1—C1—N2	-19.3 (4)	C8—C9—C14—C13	177.1 (3)
Cd1—O1—C1—C2	160.3 (2)	C19—N3—C15—C16	2.3 (6)
N1—N2—C1—O1	2.6 (5)	Cd1—N3—C15—C16	-172.4 (3)
N1—N2—C1—C2	-177.0 (3)	N3—C15—C16—C17	-2.1 (6)
O1—C1—C2—C7	-1.1 (5)	C15—C16—C17—C18	0.6 (6)
N2—C1—C2—C7	178.5 (3)	C16—C17—C18—C19	0.5 (6)
O1—C1—C2—C3	-178.0 (3)	C15—N3—C19—C18	-1.2 (6)
N2—C1—C2—C3	1.6 (5)	Cd1—N3—C19—C18	173.5 (3)
C7—C2—C3—O2	179.6 (3)	C17—C18—C19—N3	-0.2 (7)
C1—C2—C3—O2	-3.5 (5)		

Symmetry codes: (i) $-x+2, -x+y+1, -z+4/3$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O4—H4 \cdots O3	0.82	1.92	2.638 (4)	145
N2—H2 \cdots O2	0.86	1.94	2.624 (4)	135
O2—H2A \cdots O3 ⁱⁱ	0.82	1.88	2.639 (3)	153

Symmetry codes: (ii) $x-y, -y, -z+5/3$.

Fig. 1

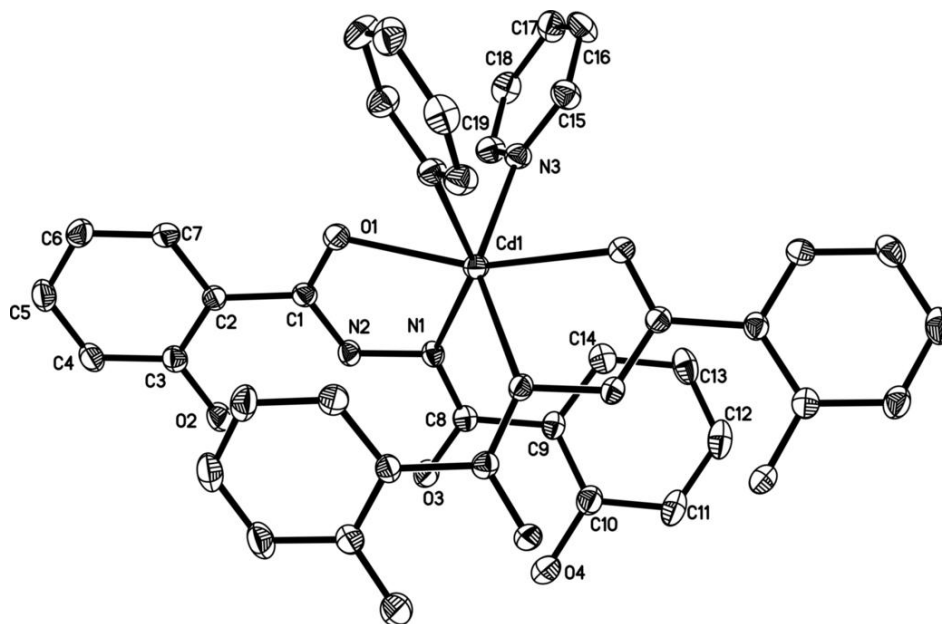


Fig. 2

