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Bis(acetato-κO)bis(2-pyridinealdoxime-$\kappa^2 N,N'$)cadmium

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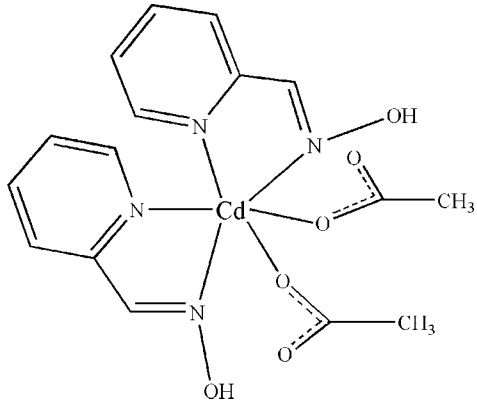
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.034; wR factor = 0.084; data-to-parameter ratio = 14.9.

In the title molecule, $[Cd(CH_3COO)_2(C_6H_6N_2O)_2]$, the Cd^{II} cation is N,N'-chelated by two 2-pyridinealdoxime ligands and coordinated by two acetate anions in a distorted octahedral geometry. The hydroxy groups of the 2-pyridinealdoxime ligands link to the acetate anions *via* intramolecular O—H···O hydrogen bonds. Weak intermolecular C—H···O hydrogen bonds occur in the crystal.

Related literature

For related structures, see: Abu-Youssef *et al.* (2010); Costa *et al.* (2009); Ha (2010); Konidaris *et al.* (2010); Korpi *et al.* (2005); Milios *et al.* (2004); Mukherjee *et al.*(2009); Torabi *et al.* (2005).



Experimental

Crystal data

$[Cd(C_2H_3O_2)_2(C_6H_6N_2O)_2]$
M_r = 474.75
Triclinic, $P\overline{1}$
a = 8.7875 (6) Å
b = 9.0946 (6) Å
c = 13.8873 (11) Å
α = 100.837 (6)°
β = 97.994 (6)°
γ = 114.700 (5)°
V = 960.42 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 298 K
0.48 × 0.38 × 0.30 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.621, T_{max} = 0.751
8165 measured reflections
3758 independent reflections
3236 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.084
S = 0.99
3758 reflections
252 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N1	2.438 (3)	Cd1—N4	2.344 (3)
Cd1—N2	2.362 (3)	Cd1—O3	2.245 (3)
Cd1—N3	2.411 (3)	Cd1—O5	2.210 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O6	0.83 (2)	1.72 (1)	2.545 (4)	169 (4)
O2—H2B···O4	0.83 (5)	1.69 (5)	2.512 (5)	175 (6)
C6—H6A···O3^{i}	0.93	2.52	3.381 (5)	153
C9—H9···O5^{ii}	0.93	2.55	3.387 (6)	151
C12—H12A···O6^{iii}	0.93	2.56	3.264 (6)	132

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5584).

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supplementary materials

Acta Cryst. (2012). E**68**, m1080–m1081 [doi:10.1107/S1600536812031819]

Bis(acetato-κO)bis(2-pyridinealdoxime-$\kappa^2 N,N'$)cadmium

Sadif A. Shirvan and Sara Haydari Dezfuli

Comment

2-Pyridinealdoxime (pya), is a good bidentate ligand, and numerous complexes with pya have been prepared, such as that of manganese (Ha, 2010; Milios *et al.*, 2004), rhenium (Costa *et al.*, 2009), nickel (Mukherjee, *et al.*, 2009), silver (Abu-Youssef *et al.*, 2010), mercury (Torabi *et al.*, 2005), zinc (Konidaris *et al.*, 2010) and copper (Korpi *et al.*, 2005). Here, we report the synthesis and structure of the title compound.

In the molecule of the title compound, (Fig. 1), the Cd^{II} atom is six-coordinated in a distorted octahedral configurations by four N atoms from two 2-pyridinealdoxime ligands and two O atom from two acetate anions. The Cd—O and Cd—N bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular O—H···O and C—H···O hydrogen bonds form a three-dimensional network (Table 2 & Fig. 2).

Experimental

A solution of 2-pyridinealdoxime (0.50 g, 4.0 mmol) in methanol (15 ml) was added to a solution of $Cd(OAc)_2.2H_2O$ (0.54 g, 2.0 mmol) in methanol (15 ml) and the resulting colorless solution was stirred for 15 min at room temperature. This solution was left to evaporate slowly at room temperature. After one week, colorless prismatic crystals of the title compound were isolated (yield 0.69 g, 72.7%).

Refinement

Hydroxyl H atoms were located in a difference Fourier map and refined isotropically. Other H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å and constrained to ride on their parent atoms with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{iso}(C)$ for the others.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Sheldrick, 2008).

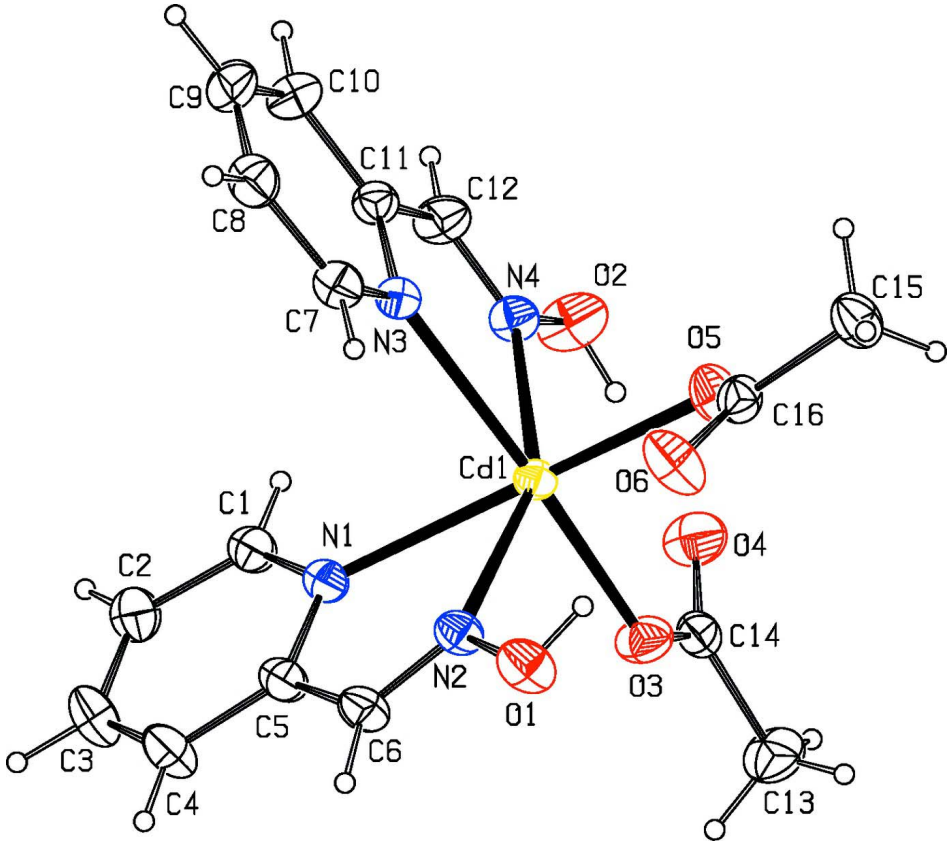

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

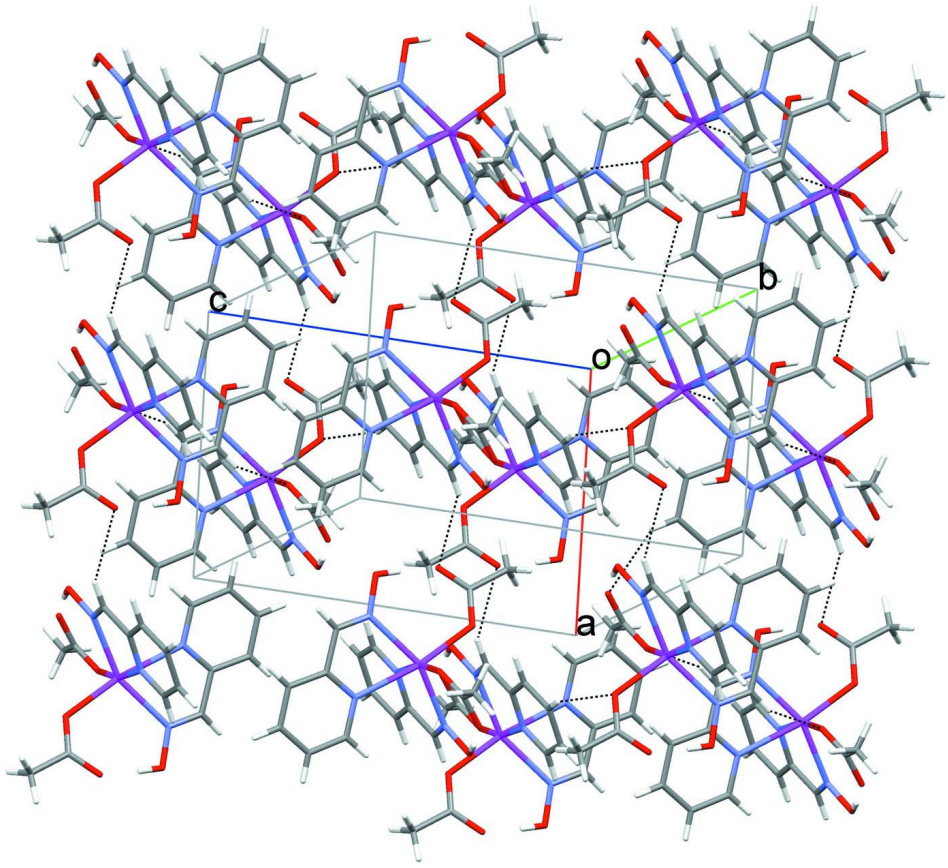

Figure 2

Unit-cell packing diagram for title compound.

Bis(acetato-κO)bis(2-pyridinealdoxime-$\kappa^2 N,N'$)cadmium(II)

Crystal data

$[Cd(C_2H_3O_2)_2(C_6H_6N_2O)_2]$
$M_r = 474.75$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.7875$ (6) Å
$b = 9.0946$ (6) Å
$c = 13.8873$ (11) Å
$\alpha = 100.837$ (6)°
$\beta = 97.994$ (6)°
$\gamma = 114.700$ (5)°
$V = 960.42$ (12) Å^3
$Z = 2$
$F(000) = 476$
$D_x = 1.642$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8165 reflections
$\theta = 1.5$–26.0°
$\mu = 1.18$ mm^{-1}
$T = 298$ K
Prism, colorless
0.48 × 0.38 × 0.30 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.621$, $T_{max} = 0.751$
8165 measured reflections
3758 independent reflections
3236 reflections with $I > 2\sigma(I)$

R_{int} = 0.056
θ_{max} = 26.0°, θ_{min} = 1.5°
h = −10→10
k = −11→11
l = −17→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.084
S = 0.99
3758 reflections
252 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 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}
C1	0.8192 (5)	0.7991 (5)	0.9158 (3)	0.0581 (9)
H1	0.8759	0.8033	0.8639	0.070*
C2	0.8947 (6)	0.7893 (6)	1.0068 (3)	0.0722 (12)
H2	0.9992	0.7843	1.0152	0.087*
C3	0.8151 (6)	0.7869 (7)	1.0838 (4)	0.0845 (14)
H3	0.8653	0.7822	1.1460	0.101*
C4	0.6590 (6)	0.7916 (7)	1.0692 (3)	0.0781 (13)
H4	0.6029	0.7915	1.1213	0.094*
C5	0.5877 (5)	0.7965 (5)	0.9757 (3)	0.0570 (9)
C6	0.4177 (5)	0.7942 (5)	0.9549 (3)	0.0601 (9)
H6A	0.3628	0.8031	1.0067	0.072*
C7	0.3108 (5)	0.3972 (5)	0.6895 (3)	0.0564 (9)
H7	0.2298	0.4142	0.7203	0.068*
C8	0.2865 (6)	0.2340 (5)	0.6552 (3)	0.0672 (11)
H8	0.1925	0.1439	0.6637	0.081*
C9	0.4040 (6)	0.2086 (5)	0.6088 (4)	0.0731 (12)
H9	0.3917	0.1006	0.5853	0.088*
C10	0.5391 (6)	0.3433 (5)	0.5972 (3)	0.0686 (11)
H10	0.6188	0.3277	0.5643	0.082*
C11	0.5577 (4)	0.5027 (5)	0.6342 (3)	0.0508 (8)
C12	0.7043 (5)	0.6520 (5)	0.6258 (3)	0.0649 (11)
H12A	0.7859	0.6391	0.5939	0.078*

C13	0.8125 (7)	1.3947 (5)	0.8418 (4)	0.0858 (14)
H13A	0.8408	1.4150	0.9139	0.103*
H13B	0.7162	1.4160	0.8218	0.103*
H13C	0.9102	1.4682	0.8214	0.103*
C14	0.7660 (5)	1.2150 (5)	0.7920 (3)	0.0560 (9)
C15	0.0811 (5)	0.7410 (6)	0.4978 (3)	0.0698 (11)
H15A	0.1029	0.6727	0.4453	0.084*
H15B	0.1167	0.8513	0.4882	0.084*
H15C	−0.0400	0.6904	0.4955	0.084*
C16	0.1808 (5)	0.7544 (5)	0.5986 (3)	0.0540 (9)
N1	0.6675 (4)	0.8026 (4)	0.8998 (2)	0.0509 (7)
N2	0.3474 (4)	0.7801 (4)	0.8656 (2)	0.0520 (7)
N3	0.4438 (3)	0.5309 (3)	0.6806 (2)	0.0459 (6)
N4	0.7206 (4)	0.7966 (4)	0.6613 (2)	0.0519 (7)
O1	0.1873 (4)	0.7749 (5)	0.8529 (2)	0.0717 (8)
H1B	0.159 (5)	0.763 (5)	0.7912 (10)	0.058 (12)*
O2	0.8603 (4)	0.9252 (4)	0.6470 (3)	0.0863 (10)
H2B	0.864 (7)	1.016 (4)	0.675 (4)	0.11 (2)*
O3	0.6409 (4)	1.1036 (3)	0.8110 (2)	0.0700 (8)
O4	0.8568 (4)	1.1901 (4)	0.7372 (3)	0.0850 (9)
O5	0.3410 (3)	0.8162 (4)	0.6126 (2)	0.0682 (7)
O6	0.0997 (4)	0.7014 (5)	0.6609 (2)	0.0892 (10)
Cd1	0.51653 (3)	0.82333 (3)	0.745759 (18)	0.04330 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.062 (2)	0.063 (2)	0.051 (2)	0.0298 (19)	0.0140 (17)	0.0144 (18)
C2	0.072 (3)	0.082 (3)	0.066 (3)	0.042 (2)	0.006 (2)	0.019 (2)
C3	0.088 (3)	0.109 (4)	0.055 (3)	0.044 (3)	0.002 (2)	0.032 (3)
C4	0.087 (3)	0.106 (4)	0.045 (2)	0.045 (3)	0.015 (2)	0.026 (2)
C5	0.064 (2)	0.061 (2)	0.0416 (19)	0.0260 (18)	0.0115 (16)	0.0115 (17)
C6	0.066 (2)	0.073 (3)	0.046 (2)	0.032 (2)	0.0223 (17)	0.0176 (18)
C7	0.0511 (19)	0.058 (2)	0.054 (2)	0.0191 (17)	0.0148 (16)	0.0152 (18)
C8	0.069 (2)	0.054 (2)	0.064 (3)	0.0150 (19)	0.012 (2)	0.019 (2)
C9	0.088 (3)	0.048 (2)	0.077 (3)	0.030 (2)	0.012 (2)	0.013 (2)
C10	0.076 (3)	0.062 (2)	0.074 (3)	0.040 (2)	0.023 (2)	0.009 (2)
C11	0.0512 (18)	0.055 (2)	0.0488 (19)	0.0270 (16)	0.0140 (15)	0.0122 (16)
C12	0.060 (2)	0.071 (3)	0.074 (3)	0.034 (2)	0.036 (2)	0.018 (2)
C13	0.098 (3)	0.047 (2)	0.095 (4)	0.020 (2)	0.022 (3)	0.010 (2)
C14	0.065 (2)	0.053 (2)	0.045 (2)	0.0239 (18)	0.0067 (17)	0.0140 (17)
C15	0.062 (2)	0.092 (3)	0.059 (2)	0.038 (2)	0.0087 (19)	0.024 (2)
C16	0.051 (2)	0.055 (2)	0.057 (2)	0.0275 (17)	0.0068 (16)	0.0141 (17)
N1	0.0543 (16)	0.0539 (17)	0.0436 (16)	0.0251 (14)	0.0106 (13)	0.0112 (13)
N2	0.0485 (15)	0.0629 (19)	0.0475 (17)	0.0252 (14)	0.0201 (13)	0.0163 (14)
N3	0.0439 (14)	0.0479 (16)	0.0434 (15)	0.0199 (12)	0.0110 (11)	0.0097 (12)
N4	0.0469 (15)	0.0542 (17)	0.0562 (17)	0.0202 (13)	0.0243 (13)	0.0174 (14)
O1	0.0535 (15)	0.110 (2)	0.0619 (19)	0.0426 (16)	0.0251 (13)	0.0259 (18)
O2	0.0739 (19)	0.064 (2)	0.123 (3)	0.0204 (16)	0.064 (2)	0.026 (2)
O3	0.0821 (19)	0.0466 (15)	0.0721 (18)	0.0207 (14)	0.0283 (15)	0.0095 (14)

O4	0.094 (2)	0.0665 (19)	0.092 (2)	0.0296 (17)	0.0422 (19)	0.0197 (18)
O5	0.0527 (15)	0.088 (2)	0.0659 (18)	0.0314 (14)	0.0095 (12)	0.0301 (16)
O6	0.0664 (18)	0.136 (3)	0.0616 (18)	0.0385 (19)	0.0151 (15)	0.038 (2)
Cd1	0.04362 (14)	0.04697 (15)	0.04136 (15)	0.02141 (11)	0.01461 (9)	0.01174 (10)

Geometric parameters (Å, º)

C1—N1	1.335 (5)	C12—N4	1.254 (5)
C1—C2	1.379 (6)	C12—H12A	0.9300
C1—H1	0.9300	C13—C14	1.502 (6)
C2—C3	1.357 (7)	C13—H13A	0.9600
C2—H2	0.9300	C13—H13B	0.9600
C3—C4	1.378 (7)	C13—H13C	0.9600
C3—H3	0.9300	C14—O4	1.235 (5)
C4—C5	1.377 (6)	C14—O3	1.246 (5)
C4—H4	0.9300	C15—C16	1.499 (5)
C5—N1	1.342 (5)	C15—H15A	0.9600
C5—C6	1.472 (5)	C15—H15B	0.9600
C6—N2	1.263 (5)	C15—H15C	0.9600
C6—H6A	0.9300	C16—O6	1.237 (5)
C7—N3	1.330 (5)	C16—O5	1.248 (4)
C7—C8	1.384 (6)	N2—O1	1.373 (4)
C7—H7	0.9300	N4—O2	1.367 (4)
C8—C9	1.366 (6)	O1—H1B	0.830 (10)
C8—H8	0.9300	O2—H2B	0.83 (5)
C9—C10	1.359 (6)	Cd1—N1	2.438 (3)
C9—H9	0.9300	Cd1—N2	2.362 (3)
C10—C11	1.376 (5)	Cd1—N3	2.411 (3)
C10—H10	0.9300	Cd1—N4	2.344 (3)
C11—N3	1.346 (4)	Cd1—O3	2.245 (3)
C11—C12	1.468 (6)	Cd1—O5	2.210 (3)
N1—C1—C2	122.3 (4)	O4—C14—C13	117.2 (4)
N1—C1—H1	118.8	O3—C14—C13	117.3 (4)
C2—C1—H1	118.8	C16—C15—H15A	109.5
C3—C2—C1	119.3 (4)	C16—C15—H15B	109.5
C3—C2—H2	120.3	H15A—C15—H15B	109.5
C1—C2—H2	120.3	C16—C15—H15C	109.5
C2—C3—C4	119.4 (4)	H15A—C15—H15C	109.5
C2—C3—H3	120.3	H15B—C15—H15C	109.5
C4—C3—H3	120.3	O6—C16—O5	124.8 (4)
C5—C4—C3	118.6 (4)	O6—C16—C15	118.3 (3)
C5—C4—H4	120.7	O5—C16—C15	116.9 (4)
C3—C4—H4	120.7	C1—N1—C5	118.0 (3)
N1—C5—C4	122.4 (4)	C1—N1—Cd1	127.0 (2)
N1—C5—C6	116.9 (3)	C5—N1—Cd1	115.0 (2)
C4—C5—C6	120.7 (4)	C6—N2—O1	115.0 (3)
N2—C6—C5	119.1 (3)	C6—N2—Cd1	118.9 (2)
N2—C6—H6A	120.4	O1—N2—Cd1	124.7 (2)
C5—C6—H6A	120.4	C7—N3—C11	117.1 (3)

N3—C7—C8	123.4 (4)	C7—N3—Cd1	127.8 (2)
N3—C7—H7	118.3	C11—N3—Cd1	115.0 (2)
C8—C7—H7	118.3	C12—N4—O2	115.3 (3)
C9—C8—C7	118.3 (4)	C12—N4—Cd1	118.4 (2)
C9—C8—H8	120.8	O2—N4—Cd1	126.3 (2)
C7—C8—H8	120.8	N2—O1—H1B	103 (3)
C10—C9—C8	119.2 (4)	N4—O2—H2B	109 (4)
C10—C9—H9	120.4	C14—O3—Cd1	129.1 (3)
C8—C9—H9	120.4	C16—O5—Cd1	124.6 (3)
C9—C10—C11	119.7 (4)	O5—Cd1—O3	95.55 (12)
C9—C10—H10	120.1	O5—Cd1—N4	96.42 (11)
C11—C10—H10	120.1	O3—Cd1—N4	100.57 (11)
N3—C11—C10	122.1 (4)	O5—Cd1—N2	103.25 (10)
N3—C11—C12	116.3 (3)	O3—Cd1—N2	91.65 (11)
C10—C11—C12	121.5 (3)	N4—Cd1—N2	155.72 (12)
N4—C12—C11	120.8 (3)	O5—Cd1—N3	92.09 (11)
N4—C12—H12A	119.6	O3—Cd1—N3	168.11 (10)
C11—C12—H12A	119.6	N4—Cd1—N3	69.45 (10)
C14—C13—H13A	109.5	N2—Cd1—N3	95.46 (10)
C14—C13—H13B	109.5	O5—Cd1—N1	170.71 (10)
H13A—C13—H13B	109.5	O3—Cd1—N1	89.02 (11)
C14—C13—H13C	109.5	N4—Cd1—N1	90.68 (10)
H13A—C13—H13C	109.5	N2—Cd1—N1	68.45 (10)
H13B—C13—H13C	109.5	N3—Cd1—N1	84.77 (10)
O4—C14—O3	125.5 (4)		

N1—C1—C2—C3	−1.5 (7)	C14—O3—Cd1—N3	43.8 (7)
C1—C2—C3—C4	1.0 (8)	C14—O3—Cd1—N1	102.2 (4)
C2—C3—C4—C5	0.8 (8)	C12—N4—Cd1—O5	−92.2 (3)
C3—C4—C5—N1	−2.3 (7)	O2—N4—Cd1—O5	88.5 (3)
C3—C4—C5—C6	177.3 (4)	C12—N4—Cd1—O3	170.9 (3)
N1—C5—C6—N2	7.4 (6)	O2—N4—Cd1—O3	−8.4 (3)
C4—C5—C6—N2	−172.3 (4)	C12—N4—Cd1—N2	51.9 (4)
N3—C7—C8—C9	−0.9 (6)	O2—N4—Cd1—N2	−127.4 (4)
C7—C8—C9—C10	−0.4 (7)	C12—N4—Cd1—N3	−2.4 (3)
C8—C9—C10—C11	1.4 (7)	O2—N4—Cd1—N3	178.3 (4)
C9—C10—C11—N3	−1.2 (7)	C12—N4—Cd1—N1	81.8 (3)
C9—C10—C11—C12	178.3 (4)	O2—N4—Cd1—N1	−97.5 (3)
N3—C11—C12—N4	0.6 (6)	C6—N2—Cd1—O5	−172.9 (3)
C10—C11—C12—N4	−178.9 (4)	O1—N2—Cd1—O5	−7.2 (3)
C2—C1—N1—C5	0.1 (6)	C6—N2—Cd1—O3	−76.8 (3)
C2—C1—N1—Cd1	179.1 (3)	O1—N2—Cd1—O3	88.9 (3)
C4—C5—N1—C1	1.9 (6)	C6—N2—Cd1—N4	43.8 (5)
C6—C5—N1—C1	−177.8 (3)	O1—N2—Cd1—N4	−150.5 (3)
C4—C5—N1—Cd1	−177.3 (4)	C6—N2—Cd1—N3	93.6 (3)
C6—C5—N1—Cd1	3.0 (4)	O1—N2—Cd1—N3	−100.7 (3)
C5—C6—N2—O1	178.4 (3)	C6—N2—Cd1—N1	11.5 (3)
C5—C6—N2—Cd1	−14.5 (5)	O1—N2—Cd1—N1	177.2 (3)
C8—C7—N3—C11	1.1 (5)	C7—N3—Cd1—O5	−84.9 (3)

C8—C7—N3—Cd1	−175.4 (3)	C11—N3—Cd1—O5	98.6 (2)
C10—C11—N3—C7	0.0 (5)	C7—N3—Cd1—O3	145.1 (5)
C12—C11—N3—C7	−179.5 (3)	C11—N3—Cd1—O3	−31.4 (6)
C10—C11—N3—Cd1	176.9 (3)	C7—N3—Cd1—N4	179.1 (3)
C12—C11—N3—Cd1	−2.6 (4)	C11—N3—Cd1—N4	2.6 (2)
C11—C12—N4—O2	−178.7 (4)	C7—N3—Cd1—N2	18.7 (3)
C11—C12—N4—Cd1	2.0 (5)	C11—N3—Cd1—N2	−157.8 (2)
O4—C14—O3—Cd1	−6.0 (6)	C7—N3—Cd1—N1	86.4 (3)
C13—C14—O3—Cd1	175.2 (3)	C11—N3—Cd1—N1	−90.1 (2)
O6—C16—O5—Cd1	6.3 (6)	C1—N1—Cd1—O5	146.5 (6)
C15—C16—O5—Cd1	−172.3 (3)	C5—N1—Cd1—O5	−34.4 (7)
C16—O5—Cd1—O3	−111.5 (3)	C1—N1—Cd1—O3	−93.9 (3)
C16—O5—Cd1—N4	147.2 (3)	C5—N1—Cd1—O3	85.2 (3)
C16—O5—Cd1—N2	−18.5 (3)	C1—N1—Cd1—N4	6.7 (3)
C16—O5—Cd1—N3	77.6 (3)	C5—N1—Cd1—N4	−174.3 (3)
C16—O5—Cd1—N1	7.6 (8)	C1—N1—Cd1—N2	173.9 (3)
C14—O3—Cd1—O5	−85.9 (4)	C5—N1—Cd1—N2	−7.0 (3)
C14—O3—Cd1—N4	11.7 (4)	C1—N1—Cd1—N3	76.0 (3)
C14—O3—Cd1—N2	170.6 (3)	C5—N1—Cd1—N3	−105.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*B*···O6	0.83 (2)	1.72 (1)	2.545 (4)	169 (4)
O2—H2*B*···O4	0.83 (5)	1.69 (5)	2.512 (5)	175 (6)
C6—H6*A*···O3^{i}	0.93	2.52	3.381 (5)	153
C9—H9···O5^{ii}	0.93	2.55	3.387 (6)	151
C12—H12*A*···O6^{iii}	0.93	2.56	3.264 (6)	132

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