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# Bis(acetato-κO)bis(2-pyridinealdoxime-κ²N,N′)cadmium

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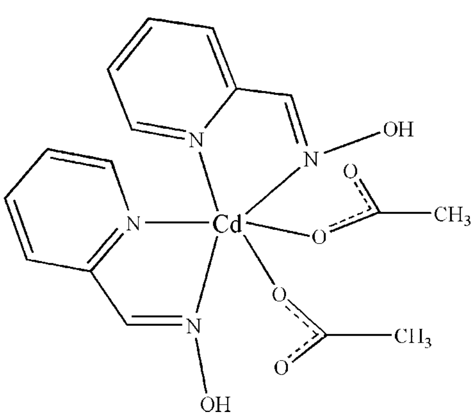
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.034; $wR$ factor = 0.084; data-to-parameter ratio = 14.9.

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, $P\bar{1}$
$a$ = 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
Mo $K\alpha$ radiation
$\mu$ = 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—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) $x+1, y, z$.

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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# supporting information

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## Bis(acetato-*κO*)bis(2-pyridinealdoxime-*κ*²*N*,*N*′)cadmium

**Sadif A. Shirvan and Sara Haydari Dezfuli**

### S1. 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).

### S2. 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%).

### S3. 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.

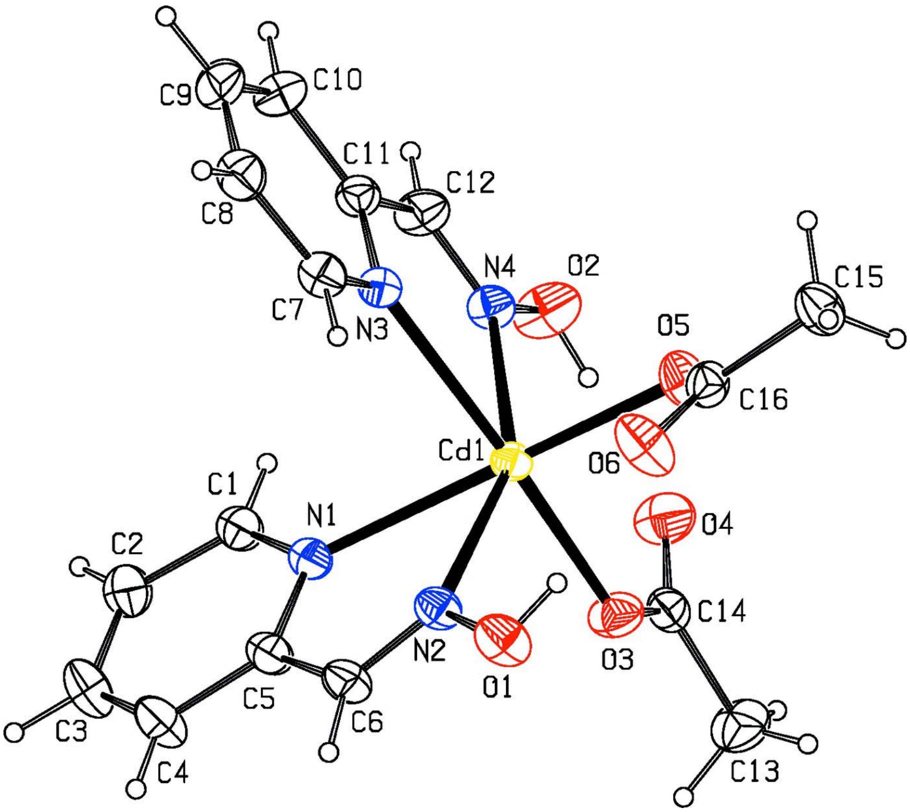


**Figure 1**

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

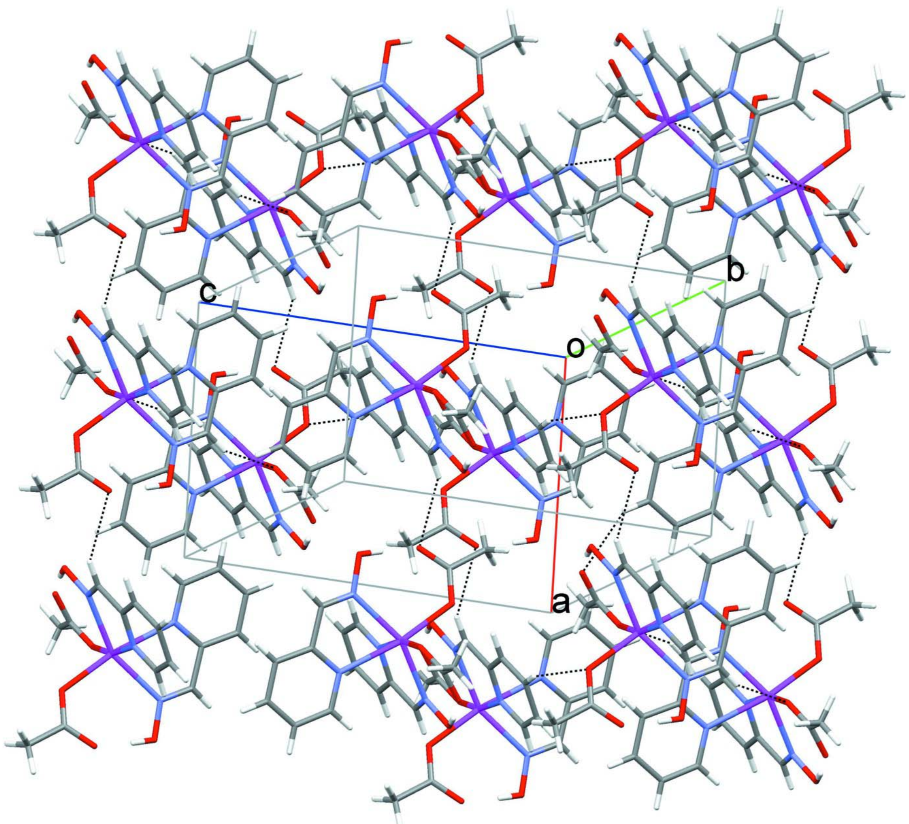


**Figure 2**

Unit-cell packing diagram for title compound.

**Bis(acetato-$\kappa O$)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
$\omega$ 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 $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.5°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 15$

*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$^{-3}$
$\Delta\rho_{min} = -0.95$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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) |

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| 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) | | |

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| 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) |

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| 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*.