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# Diaquabis(9-oxo-4,5-diazafluoren-3-olato-$\kappa^2N^4,O^3$)cadmium(II)

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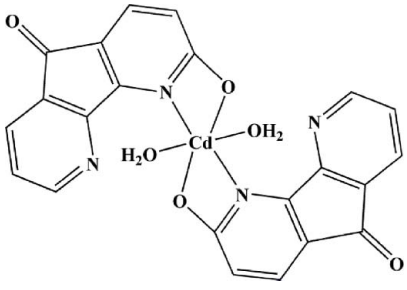
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.029; $wR$ factor = 0.082; data-to-parameter ratio = 15.2.

The title compound, $[Cd(C_{11}H_5N_2O_2)_2(H_2O)_2]$, is a mononuclear complex consisting of a $Cd^{II}$ atom, two 3-hydroxy-4,5-diazafluoren-9-one ligands and two coordinated water molecules. The $Cd^{II}$ atom, lying on a twofold axis, displays a distorted octahedral coordintion. Adjacent molecules are linked by O—H···O hydrogen bonds and $\pi$–$\pi$ interactions [centroid–centroid distance = 3.84 (1) Å], leading to a one-dimensional chain. Weak C—H···O hydrogen bonds connect the chains into a two-dimensional supramolecular structure.

## Related literature

For related literature, see: Li *et al.* (2006); Rillema *et al.* (2007); Tershansy *et al.* (2006); Zhao *et al.* (2006).




## Experimental

### Crystal data

$[Cd(C_{11}H_5N_2O_2)_2(H_2O)_2]$
$M_r$ = 542.77
Monoclinic, $C2/c$
$a$ = 28.190 (5) Å
$b$ = 5.572 (4) Å
$c$ = 13.933 (5) Å
$\beta$ = 110.622 (5)°
$V$ = 2048.3 (17) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.12 mm$^{-1}$
$T$ = 293 (2) K
0.26 × 0.21 × 0.17 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.760, $T_{max}$ = 0.833
5972 measured reflections
2406 independent reflections
1965 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.082
$S$ = 1.02
2406 reflections
158 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.233 (2) | Cd1—O2 | 2.410 (2) |
| Cd1—N1 | 2.3217 (19) | | |
| O1—Cd1—O1$^{i}$ | 101.59 (13) | O1$^{i}$—Cd1—O2 | 148.19 (7) |
| O1—Cd1—N1$^{i}$ | 92.77 (7) | N1$^{i}$—Cd1—O2 | 101.27 (7) |
| O1—Cd1—N1 | 105.03 (8) | N1—Cd1—O2 | 56.38 (7) |
| N1$^{i}$—Cd1—N1 | 151.82 (11) | O2—Cd1—O2$^{i}$ | 85.23 (11) |
| O1—Cd1—O2 | 94.62 (9) | | |

Symmetry code: (i) $-x+2, y, -z+\frac{1}{2}$.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···N2$^{i}$ | 0.82 (2) | 2.02 (2) | 2.832 (3) | 172 (3) |
| O1—H1$B$···O2$^{ii}$ | 0.83 (2) | 1.86 (2) | 2.686 (3) | 170 (4) |
| C3—H3···O3$^{iii}$ | 0.93 | 2.48 | 3.351 (5) | 156 |

Symmetry codes: (i) $-x+2, y, -z+\frac{1}{2}$; (ii) $x, y+1, z$; (iii) $-x+\frac{3}{2}, -y-\frac{1}{2}, -z$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2109).

## References

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Li, Z.-F., Wang, C.-X. & Du, C.-X. (2006). *Acta Cryst.* C**62**, m488–m490.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rillema, D. P., Kirgan, R. & Moore, C. (2007). *Acta Cryst.* E**63**, o3740.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tershansy, M. A., Goforth, A. M., Smith, M. D., Peterson, L. R. Jr & zur Loye, H.-C. (2006). *Acta Cryst.* E**62**, m3269–m3271.
Zhao, Q. H., Wang, L., Wang, K. M. & Fang, R. B. (2006). *Chin. J. Inorg. Chem.* **22**, 1285–1288.

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# supporting information

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## Diaquabis(9-oxo-4,5-diazafluoren-3-olato-$\kappa^2N^4,O^3$)cadmium(II)

**Ya-Hui Zhao, Xing Yuan, Wei-Chao Qin, Lian-Xi Sheng and Yun-Zheng Ding**

### S1. Comment

The structures of 4,5-diazafluoren-9-one and its metal complexes have been reported (Li *et al.*, 2006; Rillema *et al.*, 2007; Tershansy *et al.*, 2006; Zhao *et al.*, 2006). However, no studies of its derivative, 3-hydroxyl-4,5-diazafluoren-9-one, and any metal complexes of the ligand are known to date. In this paper, we present the crystal structure of the title compound, $[Cd(C_{11}H_5N_2O_2)_2(H_2O)_2]$.

The title compound is a neutral mononuclear complex. The $Cd^{II}$ atom is six-coordinate and exhibits a distorted octahedral coordintion geometry, defined by two N atoms and two O atoms from two 3-hydroxyl-4,5-diazafluoren-9-one ligands and two O atoms from two aqua ligands (Fig. 1). The Cd—O distances are in the range of 2.233 (2)–2.410 (2)Å and the Cd—N length is 2.322 (2) Å (Table 1). Adjacent molecules are linked by O—H···O hydrogen bonds and $\pi$–$\pi$ interactions [centroid–centroid distance 3.84 (1) Å], leading to a one-dimensional chain. Weak C—H···O hydrogen bonds connect the chains into a two-dimensional supramolecular structure (Fig. 2; Table 2).

### S2. Experimental

Cadmium(II) acetate dihydrate (0.080 g, 0.3 mmol), 3-hydroxyl-4,5-diazafluoren-9-one (0.040 g, 0.2 mmol), sodium hydroxide (0.024 g, 0.4 mmol) and water (14 ml) were placed in a 23 ml Teflon-lined autoclave, which was heated at 423 K for 3 d. After cooling slowly to room temperature at a rate of 10 K $h^{-1}$, colorless crystals of the title compound were obtained. Analysis calculated for $C_{22}H_{14}CdN_4O_6$: C 48.64, H 2.58, N 10.32%; found: C 48.51, H 2.67, N 10.42%.

### S3. Refinement

H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). H atoms of water molecule were located on a difference Fourier map and refined isotropically with a restraint of O—H = 0.82 (1) Å.

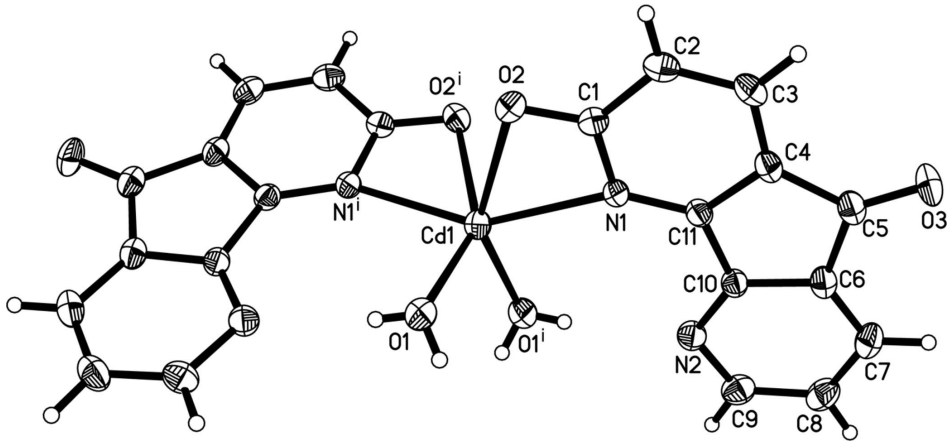


**Figure 1**

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) -*x* + 2, *y*, -*z* + 1/2.]

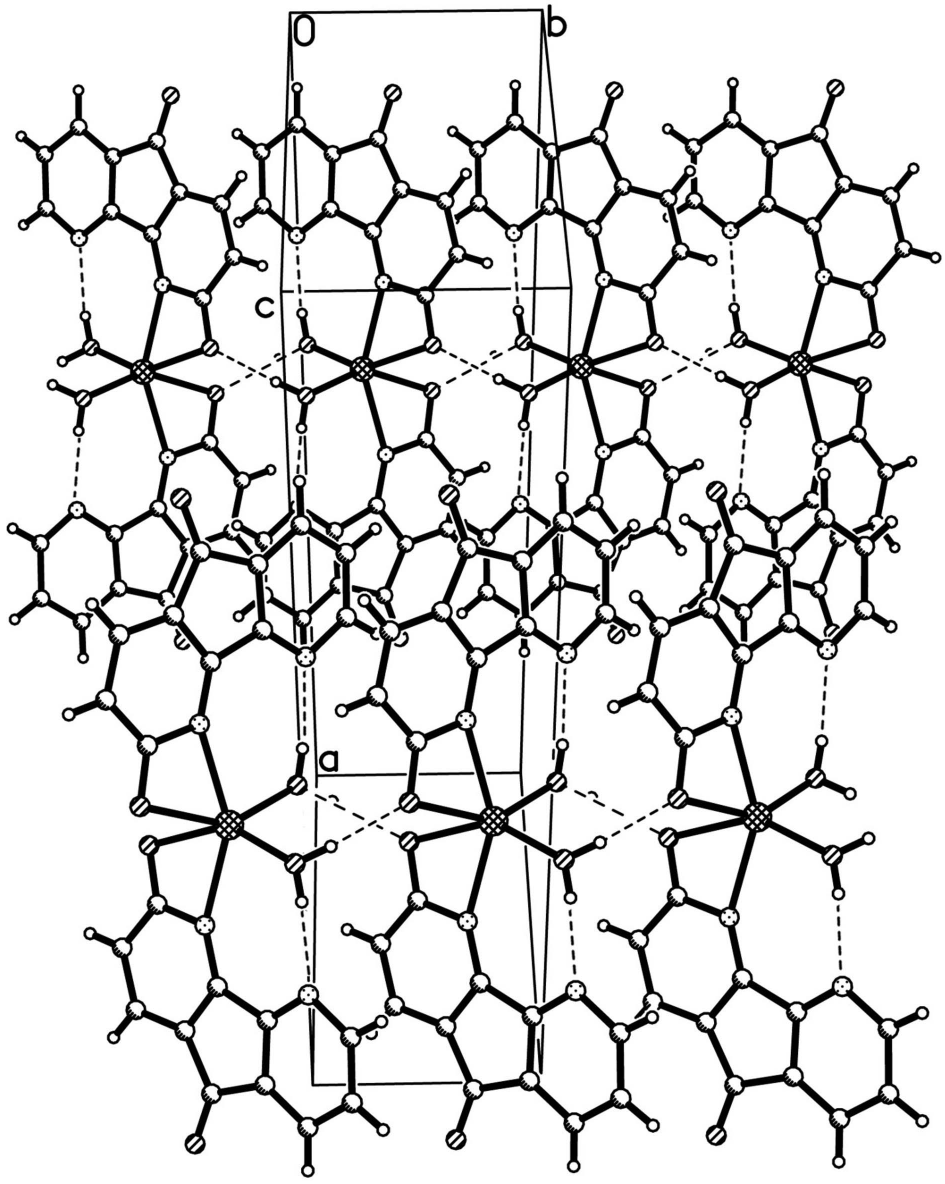


**Figure 2**

A packing diagram for the two-dimensional supramolecular structure *via* hydrogen bonds (dashed lines).

**Diaquabis(9-oxo-4,5-diazafluoren-3-olato-$\kappa^2N^4,O^3$)cadmium(II)**

*Crystal data*

$[Cd(C_{11}H_5N_2O_2)_2(H_2O)_2]$
$M_r = 542.77$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 28.190\ (5)$ Å
$b = 5.572\ (4)$ Å
$c = 13.933\ (5)$ Å
$\beta = 110.622\ (5)°$
$V = 2048.3\ (17)$ Å$^3$
$Z = 4$
$F(000) = 1080$
$D_x = 1.760$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4465 reflections
$\theta = 3.0–28.3°$
$\mu = 1.12$ mm$^{-1}$
$T = 293$ K
Block, colorless
0.26 × 0.21 × 0.17 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotation anode
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.760, $T_{max}$ = 0.833
5972 measured reflections
2406 independent reflections
1965 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 3.0°
$h$ = −26→37
$k$ = −7→7
$l$ = −18→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.082
$S$ = 1.02
2406 reflections
158 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
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 1.5483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.62 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 1.0000 | 0.24267 (5) | 0.2500 | 0.04153 (11) |
| N1 | 0.91692 (7) | 0.1412 (4) | 0.15373 (15) | 0.0337 (4) |
| N2 | 0.90481 (8) | 0.5376 (4) | −0.00770 (16) | 0.0400 (5) |
| O2 | 0.95401 (7) | −0.0756 (3) | 0.29552 (14) | 0.0455 (4) |
| O3 | 0.75172 (7) | 0.0883 (4) | −0.09790 (15) | 0.0553 (5) |
| C1 | 0.91486 (9) | −0.0461 (4) | 0.21600 (18) | 0.0358 (5) |
| C2 | 0.87029 (11) | −0.1903 (5) | 0.1904 (2) | 0.0430 (6) |
| H2 | 0.8695 | −0.3203 | 0.2317 | 0.052* |
| C3 | 0.82874 (10) | −0.1395 (5) | 0.1061 (2) | 0.0423 (6) |
| H3 | 0.7995 | −0.2322 | 0.0897 | 0.051* |
| C4 | 0.83130 (9) | 0.0555 (5) | 0.04508 (18) | 0.0366 (5) |
| C5 | 0.79449 (9) | 0.1567 (5) | −0.0489 (2) | 0.0404 (6) |
| C6 | 0.82108 (9) | 0.3654 (5) | −0.07684 (18) | 0.0377 (5) |
| C7 | 0.80569 (10) | 0.5278 (5) | −0.1560 (2) | 0.0470 (6) |
| H7 | 0.7731 | 0.5249 | −0.2045 | 0.056* |
| C8 | 0.84113 (12) | 0.6963 (5) | −0.1601 (2) | 0.0501 (7) |
| H8 | 0.8325 | 0.8102 | −0.2122 | 0.060* |
| C9 | 0.88918 (12) | 0.6950 (5) | −0.0868 (2) | 0.0460 (7) |
| H9 | 0.9122 | 0.8091 | −0.0920 | 0.055* |
| C10 | 0.87021 (9) | 0.3786 (4) | −0.00494 (17) | 0.0334 (5) |
| C11 | 0.87612 (9) | 0.1865 (4) | 0.07194 (19) | 0.0327 (5) |
| O1 | 0.99406 (8) | 0.4960 (4) | 0.36946 (16) | 0.0505 (5) |
| H1A | 1.0223 (8) | 0.519 (6) | 0.412 (2) | 0.065 (10)* |
| H1B | 0.9809 (13) | 0.630 (4) | 0.353 (3) | 0.067 (11)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.02980 (15) | 0.03837 (17) | 0.04841 (18) | 0.000 | 0.00383 (11) | 0.000 |
| N1 | 0.0281 (10) | 0.0314 (10) | 0.0377 (11) | −0.0028 (8) | 0.0066 (8) | 0.0013 (9) |
| N2 | 0.0387 (11) | 0.0401 (12) | 0.0400 (11) | −0.0032 (9) | 0.0125 (9) | 0.0036 (9) |
| O2 | 0.0427 (10) | 0.0407 (10) | 0.0454 (10) | 0.0028 (8) | 0.0058 (8) | 0.0076 (8) |
| O3 | 0.0343 (10) | 0.0707 (14) | 0.0495 (11) | −0.0142 (9) | 0.0005 (8) | −0.0081 (10) |
| C1 | 0.0369 (12) | 0.0317 (12) | 0.0382 (13) | 0.0023 (10) | 0.0124 (10) | 0.0002 (10) |
| C2 | 0.0489 (16) | 0.0348 (13) | 0.0490 (15) | −0.0056 (11) | 0.0218 (13) | 0.0017 (11) |
| C3 | 0.0385 (14) | 0.0400 (14) | 0.0494 (15) | −0.0123 (11) | 0.0168 (12) | −0.0068 (12) |
| C4 | 0.0296 (11) | 0.0403 (13) | 0.0385 (13) | −0.0051 (10) | 0.0103 (10) | −0.0061 (11) |
| C5 | 0.0331 (13) | 0.0464 (14) | 0.0396 (13) | −0.0031 (11) | 0.0100 (11) | −0.0089 (12) |
| C6 | 0.0317 (12) | 0.0444 (15) | 0.0345 (12) | −0.0003 (10) | 0.0085 (10) | −0.0048 (11) |
| C7 | 0.0415 (14) | 0.0581 (17) | 0.0355 (13) | 0.0076 (12) | 0.0062 (11) | 0.0035 (12) |
| C8 | 0.0597 (18) | 0.0509 (16) | 0.0383 (14) | 0.0123 (14) | 0.0154 (13) | 0.0101 (12) |
| C9 | 0.0500 (16) | 0.0423 (15) | 0.0499 (16) | 0.0011 (12) | 0.0227 (13) | 0.0083 (12) |
| C10 | 0.0318 (11) | 0.0350 (13) | 0.0312 (11) | −0.0004 (9) | 0.0086 (9) | −0.0022 (10) |
| C11 | 0.0296 (12) | 0.0320 (12) | 0.0353 (12) | −0.0025 (9) | 0.0097 (10) | −0.0030 (10) |
| O1 | 0.0448 (12) | 0.0426 (11) | 0.0532 (12) | 0.0076 (9) | 0.0039 (10) | −0.0025 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.233 (2) | C3—C4 | 1.397 (4) |
| Cd1—O1$^{i}$ | 2.233 (2) | C3—H3 | 0.9300 |
| Cd1—N1$^{i}$ | 2.3217 (19) | C4—C11 | 1.391 (3) |
| Cd1—N1 | 2.3217 (19) | C4—C5 | 1.468 (4) |
| Cd1—O2 | 2.410 (2) | C5—C6 | 1.507 (4) |
| Cd1—O2$^{i}$ | 2.410 (2) | C6—C7 | 1.374 (4) |
| N1—C11 | 1.327 (3) | C6—C10 | 1.396 (3) |
| N1—C1 | 1.371 (3) | C7—C8 | 1.386 (4) |
| N2—C10 | 1.328 (3) | C7—H7 | 0.9300 |
| N2—C9 | 1.355 (3) | C8—C9 | 1.380 (4) |
| O2—C1 | 1.269 (3) | C8—H8 | 0.9300 |
| O3—C5 | 1.219 (3) | C9—H9 | 0.9300 |
| C1—C2 | 1.427 (4) | C10—C11 | 1.482 (4) |
| C2—C3 | 1.365 (4) | O1—H1A | 0.817 (18) |
| C2—H2 | 0.9300 | O1—H1B | 0.832 (19) |
| | | | |
| O1—Cd1—O1$^{i}$ | 101.59 (13) | C4—C3—H3 | 120.9 |
| O1—Cd1—N1$^{i}$ | 92.77 (7) | C11—C4—C3 | 118.8 (2) |
| O1$^{i}$—Cd1—N1$^{i}$ | 105.03 (8) | C11—C4—C5 | 109.1 (2) |
| O1—Cd1—N1 | 105.03 (8) | C3—C4—C5 | 132.1 (2) |
| O1$^{i}$—Cd1—N1 | 92.77 (7) | O3—C5—C4 | 128.9 (3) |
| N1$^{i}$—Cd1—N1 | 151.82 (11) | O3—C5—C6 | 125.5 (3) |
| O1—Cd1—O2 | 94.62 (9) | C4—C5—C6 | 105.5 (2) |
| O1$^{i}$—Cd1—O2 | 148.19 (7) | C7—C6—C10 | 119.6 (2) |
| N1$^{i}$—Cd1—O2 | 101.27 (7) | C7—C6—C5 | 132.1 (2) |

| | | | |
|---|---|---|---|
| N1—Cd1—O2 | 56.38 (7) | C10—C6—C5 | 108.3 (2) |
| O1—Cd1—O2$^{i}$ | 148.19 (7) | C6—C7—C8 | 116.8 (2) |
| O1$^{i}$—Cd1—O2$^{i}$ | 94.62 (9) | C6—C7—H7 | 121.6 |
| N1$^{i}$—Cd1—O2$^{i}$ | 56.38 (7) | C8—C7—H7 | 121.6 |
| N1—Cd1—O2$^{i}$ | 101.27 (7) | C9—C8—C7 | 120.0 (3) |
| O2—Cd1—O2$^{i}$ | 85.23 (11) | C9—C8—H8 | 120.0 |
| C11—N1—C1 | 118.1 (2) | C7—C8—H8 | 120.0 |
| C11—N1—Cd1 | 147.41 (17) | N2—C9—C8 | 124.0 (3) |
| C1—N1—Cd1 | 94.51 (14) | N2—C9—H9 | 118.0 |
| C10—N2—C9 | 115.1 (2) | C8—C9—H9 | 118.0 |
| C1—O2—Cd1 | 93.31 (15) | N2—C10—C6 | 124.6 (2) |
| O2—C1—N1 | 115.7 (2) | N2—C10—C11 | 127.3 (2) |
| O2—C1—C2 | 124.3 (2) | C6—C10—C11 | 108.1 (2) |
| N1—C1—C2 | 120.0 (2) | N1—C11—C4 | 124.2 (2) |
| C3—C2—C1 | 120.8 (3) | N1—C11—C10 | 126.9 (2) |
| C3—C2—H2 | 119.6 | C4—C11—C10 | 108.9 (2) |
| C1—C2—H2 | 119.6 | Cd1—O1—H1A | 109 (2) |
| C2—C3—C4 | 118.2 (2) | Cd1—O1—H1B | 120 (2) |
| C2—C3—H3 | 120.9 | H1A—O1—H1B | 107 (3) |

| | | | |
|---|---|---|---|
| O1—Cd1—N1—C11 | 93.5 (3) | C3—C4—C5—C6 | −179.4 (3) |
| O1$^{i}$—Cd1—N1—C11 | −9.3 (3) | O3—C5—C6—C7 | 2.3 (5) |
| N1$^{i}$—Cd1—N1—C11 | −139.1 (3) | C4—C5—C6—C7 | −179.5 (3) |
| O2—Cd1—N1—C11 | 179.0 (3) | O3—C5—C6—C10 | −176.9 (3) |
| O2$^{i}$—Cd1—N1—C11 | −104.6 (3) | C4—C5—C6—C10 | 1.4 (3) |
| O1—Cd1—N1—C1 | −87.51 (16) | C10—C6—C7—C8 | 0.9 (4) |
| O1$^{i}$—Cd1—N1—C1 | 169.70 (14) | C5—C6—C7—C8 | −178.2 (3) |
| N1$^{i}$—Cd1—N1—C1 | 39.89 (13) | C6—C7—C8—C9 | 0.1 (4) |
| O2—Cd1—N1—C1 | −2.01 (13) | C10—N2—C9—C8 | 0.3 (4) |
| O2$^{i}$—Cd1—N1—C1 | 74.44 (15) | C7—C8—C9—N2 | −0.7 (5) |
| O1—Cd1—O2—C1 | 107.16 (15) | C9—N2—C10—C6 | 0.7 (4) |
| O1$^{i}$—Cd1—O2—C1 | −13.7 (2) | C9—N2—C10—C11 | −179.8 (2) |
| N1$^{i}$—Cd1—O2—C1 | −159.08 (14) | C7—C6—C10—N2 | −1.3 (4) |
| N1—Cd1—O2—C1 | 2.17 (14) | C5—C6—C10—N2 | 178.0 (2) |
| O2$^{i}$—Cd1—O2—C1 | −104.75 (16) | C7—C6—C10—C11 | 179.0 (2) |
| Cd1—O2—C1—N1 | −3.4 (2) | C5—C6—C10—C11 | −1.7 (3) |
| Cd1—O2—C1—C2 | 177.7 (2) | C1—N1—C11—C4 | −0.2 (4) |
| C11—N1—C1—O2 | −177.1 (2) | Cd1—N1—C11—C4 | 178.7 (2) |
| Cd1—N1—C1—O2 | 3.5 (2) | C1—N1—C11—C10 | −180.0 (2) |
| C11—N1—C1—C2 | 1.9 (3) | Cd1—N1—C11—C10 | −1.1 (5) |
| Cd1—N1—C1—C2 | −177.5 (2) | C3—C4—C11—N1 | −1.3 (4) |
| O2—C1—C2—C3 | 176.7 (2) | C5—C4—C11—N1 | 179.7 (2) |
| N1—C1—C2—C3 | −2.2 (4) | C3—C4—C11—C10 | 178.6 (2) |
| C1—C2—C3—C4 | 0.7 (4) | C5—C4—C11—C10 | −0.5 (3) |
| C2—C3—C4—C11 | 0.9 (4) | N2—C10—C11—N1 | 1.6 (4) |
| C2—C3—C4—C5 | 179.7 (3) | C6—C10—C11—N1 | −178.8 (2) |
| C11—C4—C5—O3 | 177.7 (3) | N2—C10—C11—C4 | −178.3 (2) |

| | | | |
|---|---|---|---|
| C3—C4—C5—O3 | −1.2 (5) | C6—C10—C11—C4 | 1.4 (3) |
| C11—C4—C5—C6 | −0.5 (3) | | |

Symmetry code: (i) −*x*+2, *y*, −*z*+1/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···N2$^{i}$ | 0.82 (2) | 2.02 (2) | 2.832 (3) | 172 (3) |
| O1—H1*B*···O2$^{ii}$ | 0.83 (2) | 1.86 (2) | 2.686 (3) | 170 (4) |
| C3—H3···O3$^{iii}$ | 0.93 | 2.48 | 3.351 (5) | 156 |

Symmetry codes: (i) −*x*+2, *y*, −*z*+1/2; (ii) *x*, *y*+1, *z*; (iii) −*x*+3/2, −*y*−1/2, −*z*.