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# *catena*-Poly[[bis($\mu_3$-5-hydroxyisophthalato)bis(pyrazino[2,3-*f*][1,10]phenanthroline)dicadmium] dihydrate]

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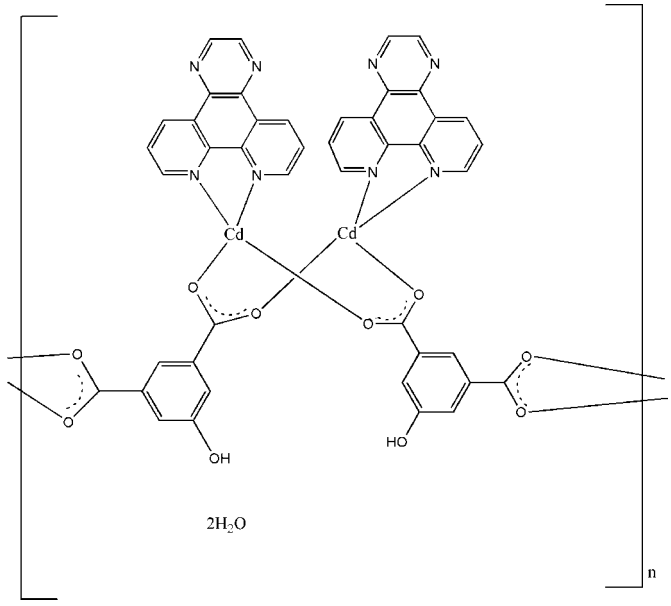
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.031; $wR$ factor = 0.114; data-to-parameter ratio = 15.6.

The title coordination polymer, $\{[Cd_2(C_8H_4O_5)_2(C_{14}H_8N_4)_2]\cdot 2H_2O\}_n$, has a layered structure. The asymmetric unit contains two $Cd^{II}$ ions, two pyrazino[2,3-*f*][1,10]phenanthroline, two 5-hydroxyisophthalate (hip) ligands and two lattice water molecules. Each $Cd^{II}$ ion is coordinated by two N atoms from a chelating pyrazino[2,3-*f*][1,10]phenanthroline and four O atoms from three different hip ligands, resulting in a distorted $CdN_2O_4$ octahedral coordination environment. The hip ligand connects adjacent $Cd^{II}$ ions, forming forming layers parallel to (010). Intralayer O—H···O hydrogen bonds involving the hydroxy groups and solvent water molecules consolidate the crystal packing.

## Related literature

For metal–carboxylate complexes containing a pyrazino[2,3-*f*][1,10]phenanthroline ligand, see: He & Han (2006); Han *et al.* (2009); Wang *et al.* (2007).




## Experimental

### Crystal data

$[Cd_2(C_8H_4O_5)_2(C_{14}H_8N_4)_2]\cdot 2H_2O$
$M_r$ = 1085.54
Triclinic, $P\overline{1}$
$a$ = 8.6754 (13) Å
$b$ = 15.1114 (17) Å
$c$ = 15.629 (3) Å
$\alpha$ = 92.903 (16)°
$\beta$ = 97.143 (13)°
$\gamma$ = 95.515 (9)°
$V$ = 2019.6 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.13 mm$^{-1}$
$T$ = 293 K
0.37 × 0.33 × 0.27 mm

### Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.681, $T_{max}$ = 0.751
11100 measured reflections
9275 independent reflections
8147 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.114
$S$ = 1.07
9275 reflections
595 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.43 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cd1—O7 | 2.205 (3) | Cd2—O2 | 2.202 (2) |
| Cd1—O1 | 2.259 (2) | Cd2—O6 | 2.295 (3) |
| Cd1—N2 | 2.339 (3) | Cd2—N5 | 2.325 (3) |
| Cd1—O4$^{i}$ | 2.360 (2) | Cd2—O9$^{ii}$ | 2.332 (2) |
| Cd1—N1 | 2.367 (3) | Cd2—N6 | 2.343 (3) |
| Cd1—O5$^{i}$ | 2.384 (3) | Cd2—O10$^{ii}$ | 2.362 (3) |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$B$···O2$W^{iii}$ | 0.82 | 1.84 | 2.659 (4) | 177 |
| O8—H8$A$···O1$W^{iv}$ | 0.82 | 1.85 | 2.672 (4) | 177 |
| O1$W$—H1$WA$···O9$^{v}$ | 0.85 | 2.14 | 2.912 (4) | 150 |
| O1$W$—H1$WB$···O2$^{v}$ | 0.85 | 2.27 | 2.963 (4) | 138 |
| O2$W$—H2$WA$···O4$^{vi}$ | 0.85 | 2.28 | 2.880 (4) | 127 |
| O2$W$—H2$WB$···O7$^{vi}$ | 0.85 | 2.33 | 2.955 (4) | 131 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2166).

## References

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m477–m478 [doi:10.1107/S1600536812011695]

## *catena*-Poly[[bis($\mu_3$-5-hydroxyisophthalato)bis(pyrazino[2,3-*f*][1,10]phenanthroline)dicadmium] dihydrate]

**Peng-Cheng Zhao**

### Comment

Recently, several metal-carboxylate complexes containing an N-donor chelate ligand TATP and its large analogue DPPZ dipyridophenazine have been reported (He & Han, 2006; Wang *et al.*, 2007; Han *et al.*, 2009). I report here a new one-dimensional $Cd^{II}$ coordination polymer constructed by $Cd^{II}$ ions, pyrazino[2,3-*f*][1,10]phenanthroline (TATP) and 5-hydroxyisophthalic acid ($H_2Hip$), (I).

Complex (I) exhibits a layered structure in which the asymmetric unit consists of two $Cd^{II}$ ions, two hip, two TATP ligand and two lattice water molecules (Fig. 1). Fig. 2 shows a fragment of the fragment of ribbon chain in the structure of I. Each $Cd^{II}$ is hexa-coordinate and is surrounded by four oxygen atoms from three different hip ligands and two nitrogen atoms from a chelating TATP ligand (Table 1), forming a distorted octahedral geometry.

The hip ligand connects adjacent $Cd^{II}$ ions, forming layers parallel to (010). Intralayer O—H···O hydrogen bonds involving the hydroxy groups and solvent water molecules consolidate the crystal packing. A face-to-face distance of 3.491 Å between a pair of TATP ligands coordinated to the two $Cd^{II}$ ions is observed, showing significant $\pi$–$\pi$ stacking interactions.

### Experimental

A mixture of $Cd(NO_3)_2.4H_2O$ (0.5 mmol, 0.154 g), pyrazino[2,3-*f*][1,10]phenanthroline ligand (0.5 mmol, 0.116 g), $H_2hip$ (0.5 mmol, 0.083 g) and water (10 ml) was mixed in a 23 ml Teflon reactor, which was heated at 180° for six days and then cooled to room temperature at a rate of 5 ° $h^{-1}$.Yield: 38%. CH&N analysis for $C_{68}H_{38}Cu_3N_8$ (found/calc): C, 48.68(48.97), H, 2.60(2.71), N, 10.32%(10.63%).

### Refinement

The H atoms of the aromatic rings were placed at calculated positions in the riding model approximation (C—H 0.93 Å) with their temperature factors were set to 1.2 times those of the equivalent isotropic temperature factors of the parent atoms. The hydroxy H atom was placed at calculated positions in the riding model approximation(O—H 0.82 Å) with their temperature factors were set to 1.2 times those of the equivalent isotropic temperature factors of the parent atoms.

### Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXL97* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

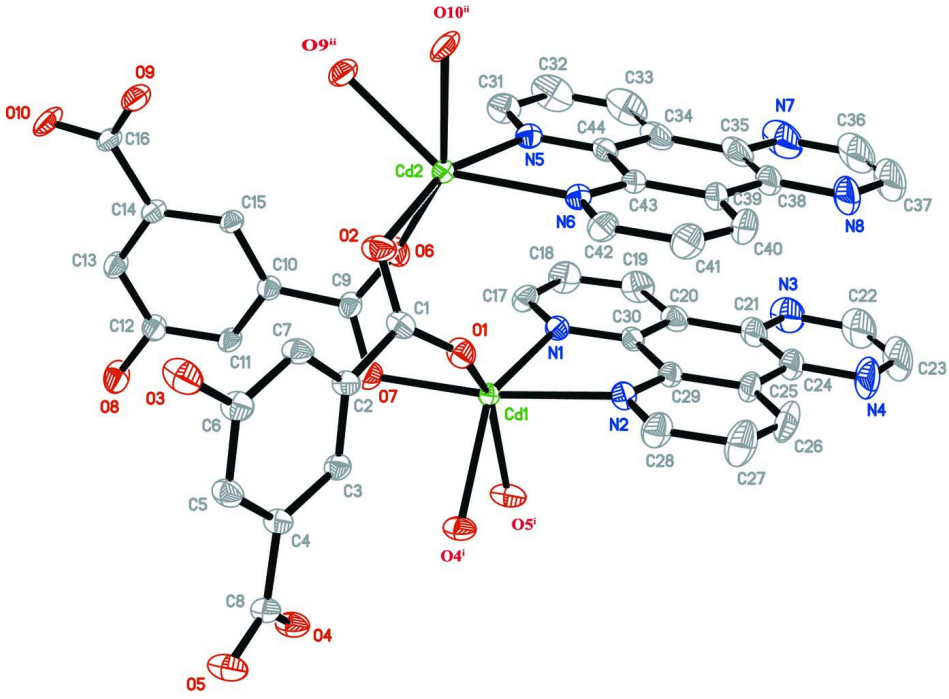


**Figure 1**

View of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms and the lattice water molecule have been omitted for clarity. [Symmetry code: (i) -*x*, -*y* + 1, -*z* + 1.]

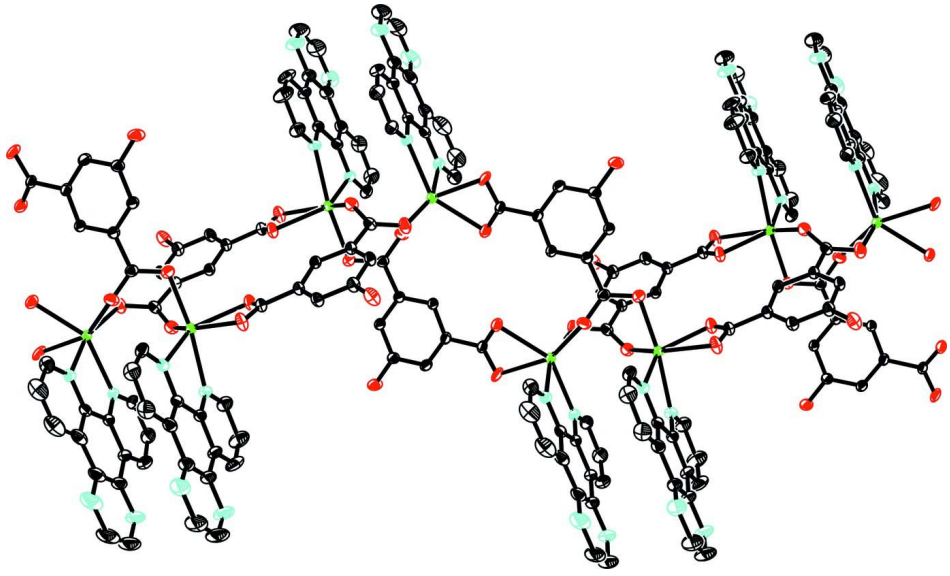

**Figure 2**

The fragment of one-dimensional ribbon chain.

**i>catena-Poly[[bis($\mu_3$-5-hydroxyisophthalato)bis(pyrazino[2,3- f][1,10]phenanthroline)dicadmium] dihydrate]**

*Crystal data*

$[Cd_2(C_8H_4O_5)_2(C_{14}H_8N_4)_2]\cdot 2H_2O$
$M_r = 1085.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.6754\ (13)$ Å
$b = 15.1114\ (17)$ Å
$c = 15.629\ (3)$ Å
$\alpha = 92.903\ (16)°$
$\beta = 97.143\ (13)°$
$\gamma = 95.515\ (9)°$
$V = 2019.6\ (5)$ Å$^3$
$Z = 2$
$F(000) = 1080$
$D_x = 1.785$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20 reflections
$\theta = 2.7–22.3°$
$\mu = 1.13$ mm$^{-1}$
$T = 293$ K
Block, red
0.37 × 0.33 × 0.27 mm

*Data collection*

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.681$, $T_{max} = 0.751$
11100 measured reflections
9275 independent reflections
8147 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.8°$
$h = -1\rightarrow 11$
$k = -19\rightarrow 19$
$l = -20\rightarrow 20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.114$
$S = 1.07$
9275 reflections
595 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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 2.6404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.70$ e Å$^{-3}$
$\Delta\rho_{min} = -1.43$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.10447 (3) | 0.188967 (14) | 0.170325 (14) | 0.02701 (8) |
| Cd2 | 0.47056 (3) | 0.185064 (14) | 0.355404 (14) | 0.02830 (8) |
| C1 | 0.4157 (4) | 0.0769 (2) | 0.1864 (2) | 0.0325 (7) |
| C2 | 0.4157 (4) | −0.0043 (2) | 0.1274 (2) | 0.0293 (6) |

| | | | | |
|---|---|---|---|---|
| C3 | 0.2868 (4) | −0.0312 (2) | 0.0662 (2) | 0.0298 (6) |
| H3A | 0.2047 | 0.0041 | 0.0578 | 0.036* |
| C4 | 0.2821 (4) | −0.1116 (2) | 0.0176 (2) | 0.0306 (6) |
| C5 | 0.4080 (4) | −0.1622 (2) | 0.0279 (2) | 0.0355 (7) |
| H5A | 0.4056 | −0.2151 | −0.0055 | 0.043* |
| C6 | 0.5372 (4) | −0.1341 (2) | 0.0879 (2) | 0.0359 (7) |
| C7 | 0.5410 (4) | −0.0553 (2) | 0.1379 (2) | 0.0327 (7) |
| H7A | 0.6272 | −0.0366 | 0.1785 | 0.039* |
| C8 | 0.1421 (4) | −0.1441 (2) | −0.0463 (2) | 0.0328 (7) |
| C9 | 0.1081 (4) | 0.0759 (2) | 0.3173 (2) | 0.0327 (7) |
| C10 | 0.0805 (4) | −0.0039 (2) | 0.3672 (2) | 0.0301 (6) |
| C11 | −0.0632 (4) | −0.0553 (2) | 0.3504 (2) | 0.0335 (7) |
| H11A | −0.1422 | −0.0371 | 0.3114 | 0.040* |
| C12 | −0.0887 (4) | −0.1337 (2) | 0.3918 (2) | 0.0355 (7) |
| C13 | 0.0304 (4) | −0.1612 (2) | 0.4484 (2) | 0.0362 (7) |
| H13A | 0.0143 | −0.2141 | 0.4755 | 0.043* |
| C14 | 0.1743 (4) | −0.1098 (2) | 0.4649 (2) | 0.0306 (6) |
| C15 | 0.1995 (4) | −0.0305 (2) | 0.4259 (2) | 0.0297 (6) |
| H15A | 0.2944 | 0.0047 | 0.4386 | 0.036* |
| C16 | 0.3017 (4) | −0.1412 (2) | 0.5267 (2) | 0.0314 (6) |
| C17 | −0.0218 (5) | 0.3044 (3) | 0.3270 (2) | 0.0407 (8) |
| H17A | −0.0325 | 0.2492 | 0.3506 | 0.049* |
| C18 | −0.0821 (6) | 0.3758 (3) | 0.3664 (3) | 0.0544 (11) |
| H18A | −0.1310 | 0.3686 | 0.4156 | 0.065* |
| C19 | −0.0680 (6) | 0.4571 (3) | 0.3312 (3) | 0.0565 (11) |
| H19A | −0.1064 | 0.5058 | 0.3568 | 0.068* |
| C20 | 0.0046 (5) | 0.4664 (2) | 0.2565 (3) | 0.0419 (8) |
| C21 | 0.0198 (5) | 0.5501 (3) | 0.2146 (3) | 0.0509 (10) |
| C22 | −0.0273 (9) | 0.6946 (3) | 0.2073 (5) | 0.090 (2) |
| H22A | −0.0683 | 0.7450 | 0.2279 | 0.108* |
| C23 | 0.0499 (9) | 0.6999 (3) | 0.1355 (6) | 0.097 (2) |
| H23A | 0.0581 | 0.7540 | 0.1098 | 0.117* |
| C24 | 0.0961 (6) | 0.5557 (3) | 0.1413 (3) | 0.0531 (11) |
| C25 | 0.1584 (5) | 0.4778 (3) | 0.1055 (3) | 0.0439 (9) |
| C26 | 0.2386 (7) | 0.4795 (4) | 0.0330 (3) | 0.0671 (14) |
| H26A | 0.2538 | 0.5320 | 0.0052 | 0.081* |
| C27 | 0.2944 (7) | 0.4036 (4) | 0.0034 (4) | 0.0712 (15) |
| H27A | 0.3496 | 0.4044 | −0.0440 | 0.085* |
| C28 | 0.2678 (5) | 0.3250 (3) | 0.0449 (3) | 0.0495 (10) |
| H28A | 0.3031 | 0.2731 | 0.0235 | 0.059* |
| C29 | 0.1410 (4) | 0.3973 (2) | 0.1447 (2) | 0.0329 (7) |
| C30 | 0.0625 (4) | 0.3913 (2) | 0.2218 (2) | 0.0317 (6) |
| C31 | 0.3204 (5) | 0.3164 (3) | 0.4855 (3) | 0.0500 (10) |
| H31A | 0.3056 | 0.2645 | 0.5143 | 0.060* |
| C32 | 0.2675 (6) | 0.3944 (4) | 0.5176 (4) | 0.0709 (15) |
| H32A | 0.2197 | 0.3945 | 0.5677 | 0.085* |
| C33 | 0.2864 (6) | 0.4703 (4) | 0.4750 (4) | 0.0718 (16) |
| H33A | 0.2503 | 0.5223 | 0.4954 | 0.086* |
| C34 | 0.3604 (5) | 0.4699 (3) | 0.4003 (3) | 0.0499 (10) |

| | | | | |
|---|---|---|---|---|
| C35 | 0.3880 (6) | 0.5474 (3) | 0.3515 (4) | 0.0602 (14) |
| C36 | 0.3659 (10) | 0.6943 (4) | 0.3319 (7) | 0.105 (3) |
| H36A | 0.3323 | 0.7486 | 0.3482 | 0.126* |
| C37 | 0.4468 (10) | 0.6902 (4) | 0.2608 (6) | 0.104 (3) |
| H37A | 0.4666 | 0.7415 | 0.2318 | 0.125* |
| C38 | 0.4669 (6) | 0.5434 (3) | 0.2791 (3) | 0.0574 (12) |
| C39 | 0.5212 (5) | 0.4600 (2) | 0.2509 (3) | 0.0457 (9) |
| C40 | 0.6034 (6) | 0.4512 (3) | 0.1801 (3) | 0.0616 (13) |
| H40A | 0.6253 | 0.5000 | 0.1481 | 0.074* |
| C41 | 0.6517 (6) | 0.3701 (3) | 0.1580 (3) | 0.0574 (11) |
| H41A | 0.7090 | 0.3641 | 0.1119 | 0.069* |
| C42 | 0.6148 (5) | 0.2978 (3) | 0.2045 (2) | 0.0419 (8) |
| H42A | 0.6449 | 0.2428 | 0.1879 | 0.050* |
| C43 | 0.4924 (4) | 0.3842 (2) | 0.2967 (2) | 0.0331 (7) |
| C44 | 0.4124 (4) | 0.3889 (2) | 0.3731 (2) | 0.0331 (7) |
| N1 | 0.0498 (3) | 0.31172 (18) | 0.25765 (18) | 0.0313 (6) |
| N2 | 0.1936 (3) | 0.32205 (19) | 0.11392 (19) | 0.0347 (6) |
| N3 | −0.0450 (6) | 0.6199 (3) | 0.2481 (3) | 0.0731 (13) |
| N4 | 0.1131 (6) | 0.6324 (3) | 0.1010 (4) | 0.0768 (14) |
| N5 | 0.3913 (3) | 0.3145 (2) | 0.41515 (18) | 0.0341 (6) |
| N6 | 0.5371 (3) | 0.30456 (19) | 0.27266 (18) | 0.0320 (6) |
| N7 | 0.3338 (6) | 0.6247 (3) | 0.3780 (4) | 0.0876 (17) |
| N8 | 0.4967 (6) | 0.6145 (3) | 0.2330 (4) | 0.0839 (16) |
| O1 | 0.3399 (3) | 0.13916 (16) | 0.16202 (18) | 0.0387 (5) |
| O2 | 0.4944 (3) | 0.07607 (18) | 0.26051 (17) | 0.0445 (6) |
| O3 | 0.6581 (3) | −0.18602 (19) | 0.0963 (2) | 0.0507 (7) |
| H3B | 0.7409 | −0.1541 | 0.1070 | 0.076* |
| O4 | 0.0151 (3) | −0.11105 (18) | −0.04066 (16) | 0.0396 (6) |
| O5 | 0.1536 (3) | −0.2029 (2) | −0.10328 (18) | 0.0463 (7) |
| O6 | 0.2090 (3) | 0.13873 (17) | 0.34703 (19) | 0.0411 (6) |
| O7 | 0.0264 (3) | 0.07608 (18) | 0.24391 (18) | 0.0452 (6) |
| O8 | −0.2273 (3) | −0.1863 (2) | 0.3755 (2) | 0.0531 (8) |
| H8A | −0.2992 | −0.1548 | 0.3689 | 0.080* |
| O9 | 0.4413 (3) | −0.10890 (18) | 0.52495 (17) | 0.0418 (6) |
| O10 | 0.2685 (3) | −0.1985 (2) | 0.57699 (19) | 0.0488 (7) |
| O1W | 0.5320 (3) | 0.9117 (2) | 0.3532 (2) | 0.0517 (7) |
| H1WA | 0.4828 | 0.9197 | 0.3963 | 0.062* |
| H1WB | 0.5729 | 0.9562 | 0.3299 | 0.062* |
| O2W | 0.9326 (3) | 0.91177 (19) | 0.1314 (2) | 0.0482 (6) |
| H2WA | 0.9958 | 0.8862 | 0.1036 | 0.058* |
| H2WB | 0.9335 | 0.9681 | 0.1328 | 0.058* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.02968 (12) | 0.02234 (12) | 0.02818 (12) | 0.00372 (8) | −0.00040 (9) | 0.00180 (8) |
| Cd2 | 0.03162 (13) | 0.02485 (12) | 0.02733 (12) | 0.00397 (9) | −0.00178 (9) | 0.00298 (8) |
| C1 | 0.0262 (15) | 0.0321 (16) | 0.0382 (17) | 0.0037 (12) | 0.0032 (13) | −0.0048 (13) |
| C2 | 0.0280 (15) | 0.0315 (15) | 0.0284 (15) | 0.0067 (12) | 0.0022 (12) | −0.0014 (12) |
| C3 | 0.0294 (15) | 0.0305 (15) | 0.0298 (15) | 0.0079 (12) | 0.0011 (12) | 0.0012 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0290 (15) | 0.0341 (16) | 0.0281 (15) | 0.0040 (12) | 0.0019 (12) | −0.0021 (12) |
| C5 | 0.0362 (17) | 0.0334 (16) | 0.0359 (17) | 0.0079 (13) | 0.0015 (14) | −0.0088 (13) |
| C6 | 0.0283 (15) | 0.0396 (18) | 0.0401 (18) | 0.0119 (13) | 0.0013 (13) | −0.0032 (14) |
| C7 | 0.0272 (15) | 0.0364 (17) | 0.0330 (16) | 0.0072 (13) | −0.0024 (12) | −0.0048 (13) |
| C8 | 0.0303 (16) | 0.0371 (17) | 0.0293 (15) | 0.0026 (13) | −0.0010 (12) | −0.0014 (13) |
| C9 | 0.0285 (15) | 0.0310 (16) | 0.0390 (17) | 0.0039 (12) | 0.0038 (13) | 0.0077 (13) |
| C10 | 0.0265 (14) | 0.0309 (15) | 0.0329 (16) | 0.0029 (12) | 0.0024 (12) | 0.0053 (12) |
| C11 | 0.0255 (15) | 0.0358 (17) | 0.0382 (17) | 0.0015 (12) | −0.0028 (13) | 0.0112 (14) |
| C12 | 0.0271 (15) | 0.0357 (17) | 0.0428 (18) | −0.0020 (13) | 0.0026 (13) | 0.0091 (14) |
| C13 | 0.0330 (16) | 0.0370 (17) | 0.0390 (18) | 0.0014 (13) | 0.0028 (14) | 0.0143 (14) |
| C14 | 0.0287 (15) | 0.0362 (16) | 0.0269 (14) | 0.0041 (12) | 0.0016 (12) | 0.0080 (12) |
| C15 | 0.0251 (14) | 0.0329 (16) | 0.0302 (15) | 0.0013 (12) | −0.0010 (12) | 0.0066 (12) |
| C16 | 0.0317 (16) | 0.0353 (16) | 0.0269 (15) | 0.0059 (13) | −0.0019 (12) | 0.0074 (12) |
| C17 | 0.049 (2) | 0.045 (2) | 0.0304 (17) | 0.0088 (16) | 0.0089 (15) | 0.0065 (14) |
| C18 | 0.066 (3) | 0.059 (3) | 0.042 (2) | 0.013 (2) | 0.022 (2) | −0.0035 (19) |
| C19 | 0.066 (3) | 0.052 (2) | 0.053 (2) | 0.019 (2) | 0.013 (2) | −0.014 (2) |
| C20 | 0.0424 (19) | 0.0328 (17) | 0.048 (2) | 0.0073 (15) | −0.0021 (16) | −0.0064 (15) |
| C21 | 0.055 (2) | 0.0277 (17) | 0.067 (3) | 0.0118 (16) | −0.009 (2) | −0.0003 (17) |
| C22 | 0.111 (5) | 0.032 (2) | 0.122 (6) | 0.030 (3) | −0.015 (4) | −0.004 (3) |
| C23 | 0.116 (6) | 0.030 (2) | 0.141 (7) | 0.017 (3) | −0.015 (5) | 0.023 (3) |
| C24 | 0.059 (3) | 0.0320 (19) | 0.065 (3) | 0.0057 (17) | −0.010 (2) | 0.0135 (18) |
| C25 | 0.047 (2) | 0.0348 (18) | 0.049 (2) | 0.0035 (15) | −0.0007 (17) | 0.0165 (16) |
| C26 | 0.082 (4) | 0.060 (3) | 0.064 (3) | 0.004 (3) | 0.019 (3) | 0.038 (2) |
| C27 | 0.087 (4) | 0.072 (3) | 0.066 (3) | 0.013 (3) | 0.041 (3) | 0.028 (3) |
| C28 | 0.057 (2) | 0.052 (2) | 0.044 (2) | 0.0081 (19) | 0.0199 (19) | 0.0089 (18) |
| C29 | 0.0320 (16) | 0.0285 (15) | 0.0371 (17) | 0.0030 (12) | −0.0003 (13) | 0.0034 (13) |
| C30 | 0.0304 (15) | 0.0273 (15) | 0.0362 (16) | 0.0024 (12) | 0.0007 (13) | 0.0001 (12) |
| C31 | 0.049 (2) | 0.061 (3) | 0.040 (2) | 0.0011 (19) | 0.0132 (17) | −0.0023 (18) |
| C32 | 0.061 (3) | 0.084 (4) | 0.069 (3) | 0.006 (3) | 0.029 (3) | −0.027 (3) |
| C33 | 0.059 (3) | 0.065 (3) | 0.091 (4) | 0.016 (2) | 0.015 (3) | −0.035 (3) |
| C34 | 0.040 (2) | 0.038 (2) | 0.067 (3) | 0.0092 (16) | −0.0071 (18) | −0.0175 (18) |
| C35 | 0.052 (2) | 0.0293 (19) | 0.090 (4) | 0.0079 (17) | −0.025 (2) | −0.010 (2) |
| C36 | 0.108 (6) | 0.027 (2) | 0.164 (8) | 0.015 (3) | −0.047 (5) | −0.005 (4) |
| C37 | 0.122 (6) | 0.029 (2) | 0.147 (7) | 0.003 (3) | −0.037 (5) | 0.018 (3) |
| C38 | 0.061 (3) | 0.0285 (18) | 0.075 (3) | 0.0010 (17) | −0.023 (2) | 0.0097 (19) |
| C39 | 0.050 (2) | 0.0318 (18) | 0.050 (2) | −0.0046 (16) | −0.0110 (17) | 0.0113 (16) |
| C40 | 0.072 (3) | 0.055 (3) | 0.054 (3) | −0.014 (2) | 0.002 (2) | 0.025 (2) |
| C41 | 0.067 (3) | 0.067 (3) | 0.038 (2) | −0.008 (2) | 0.016 (2) | 0.009 (2) |
| C42 | 0.048 (2) | 0.046 (2) | 0.0312 (17) | 0.0009 (16) | 0.0083 (15) | 0.0050 (15) |
| C43 | 0.0330 (16) | 0.0294 (15) | 0.0342 (16) | 0.0000 (12) | −0.0047 (13) | 0.0035 (13) |
| C44 | 0.0308 (16) | 0.0288 (15) | 0.0373 (17) | 0.0026 (12) | −0.0027 (13) | −0.0042 (13) |
| N1 | 0.0336 (14) | 0.0295 (13) | 0.0307 (13) | 0.0040 (11) | 0.0041 (11) | 0.0008 (11) |
| N2 | 0.0370 (15) | 0.0308 (14) | 0.0368 (15) | 0.0023 (11) | 0.0073 (12) | 0.0021 (11) |
| N3 | 0.086 (3) | 0.041 (2) | 0.091 (3) | 0.028 (2) | −0.006 (3) | −0.010 (2) |
| N4 | 0.092 (3) | 0.039 (2) | 0.101 (4) | 0.010 (2) | 0.002 (3) | 0.032 (2) |
| N5 | 0.0356 (14) | 0.0360 (15) | 0.0300 (14) | 0.0032 (12) | 0.0029 (11) | 0.0006 (11) |
| N6 | 0.0370 (15) | 0.0312 (14) | 0.0273 (13) | 0.0026 (11) | 0.0025 (11) | 0.0014 (11) |
| N7 | 0.086 (3) | 0.040 (2) | 0.129 (5) | 0.022 (2) | −0.019 (3) | −0.023 (3) |
| N8 | 0.097 (4) | 0.034 (2) | 0.110 (4) | −0.008 (2) | −0.027 (3) | 0.025 (2) |

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|---|---|---|---|---|---|---|
| O1 | 0.0341 (12) | 0.0315 (12) | 0.0504 (15) | 0.0095 (10) | 0.0017 (11) | −0.0017 (11) |
| O2 | 0.0493 (15) | 0.0424 (14) | 0.0387 (14) | 0.0153 (12) | −0.0084 (11) | −0.0117 (11) |
| O3 | 0.0348 (13) | 0.0447 (15) | 0.0699 (19) | 0.0169 (11) | −0.0047 (13) | −0.0188 (14) |
| O4 | 0.0324 (12) | 0.0468 (14) | 0.0371 (13) | 0.0101 (10) | −0.0058 (10) | −0.0080 (11) |
| O5 | 0.0378 (14) | 0.0566 (17) | 0.0409 (14) | 0.0113 (12) | −0.0061 (11) | −0.0168 (12) |
| O6 | 0.0342 (13) | 0.0321 (12) | 0.0549 (16) | −0.0020 (10) | 0.0019 (11) | 0.0042 (11) |
| O7 | 0.0449 (15) | 0.0430 (14) | 0.0442 (15) | −0.0060 (12) | −0.0050 (12) | 0.0161 (12) |
| O8 | 0.0294 (13) | 0.0476 (16) | 0.080 (2) | −0.0081 (11) | −0.0032 (13) | 0.0275 (15) |
| O9 | 0.0314 (12) | 0.0500 (15) | 0.0428 (14) | 0.0010 (11) | −0.0044 (10) | 0.0201 (12) |
| O10 | 0.0400 (14) | 0.0602 (17) | 0.0460 (15) | 0.0017 (12) | −0.0053 (11) | 0.0358 (13) |
| O1W | 0.0513 (16) | 0.0541 (17) | 0.0541 (17) | 0.0138 (13) | 0.0142 (13) | 0.0125 (14) |
| O2W | 0.0439 (15) | 0.0442 (15) | 0.0571 (17) | 0.0021 (12) | 0.0106 (13) | 0.0023 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O7 | 2.205 (3) | C21—C24 | 1.395 (7) |
| Cd1—O1 | 2.259 (2) | C22—N3 | 1.331 (8) |
| Cd1—N2 | 2.339 (3) | C22—C23 | 1.377 (11) |
| Cd1—O4$^{i}$ | 2.360 (2) | C22—H22A | 0.9300 |
| Cd1—N1 | 2.367 (3) | C23—N4 | 1.326 (9) |
| Cd1—O5$^{i}$ | 2.384 (3) | C23—H23A | 0.9300 |
| Cd1—C8$^{i}$ | 2.711 (3) | C24—N4 | 1.351 (6) |
| Cd2—O2 | 2.202 (2) | C24—C25 | 1.457 (6) |
| Cd2—O6 | 2.295 (3) | C25—C29 | 1.393 (5) |
| Cd2—N5 | 2.325 (3) | C25—C26 | 1.402 (7) |
| Cd2—O9$^{ii}$ | 2.332 (2) | C26—C27 | 1.369 (8) |
| Cd2—N6 | 2.343 (3) | C26—H26A | 0.9300 |
| Cd2—O10$^{ii}$ | 2.362 (3) | C27—C28 | 1.396 (6) |
| Cd2—C16$^{ii}$ | 2.685 (3) | C27—H27A | 0.9300 |
| C1—O1 | 1.247 (4) | C28—N2 | 1.323 (5) |
| C1—O2 | 1.271 (4) | C28—H28A | 0.9300 |
| C1—C2 | 1.497 (4) | C29—N2 | 1.353 (4) |
| C2—C7 | 1.390 (4) | C29—C30 | 1.459 (5) |
| C2—C3 | 1.392 (4) | C30—N1 | 1.353 (4) |
| C3—C4 | 1.394 (4) | C31—N5 | 1.325 (5) |
| C3—H3A | 0.9300 | C31—C32 | 1.397 (7) |
| C4—C5 | 1.391 (5) | C31—H31A | 0.9300 |
| C4—C8 | 1.499 (4) | C32—C33 | 1.362 (9) |
| C5—C6 | 1.386 (5) | C32—H32A | 0.9300 |
| C5—H5A | 0.9300 | C33—C34 | 1.400 (8) |
| C6—O3 | 1.366 (4) | C33—H33A | 0.9300 |
| C6—C7 | 1.386 (5) | C34—C44 | 1.408 (5) |
| C7—H7A | 0.9300 | C34—C35 | 1.447 (7) |
| C8—O5 | 1.245 (4) | C35—N7 | 1.365 (6) |
| C8—O4 | 1.264 (4) | C35—C38 | 1.396 (8) |
| C8—Cd1$^{i}$ | 2.711 (3) | C36—N7 | 1.332 (10) |
| C9—O6 | 1.257 (4) | C36—C37 | 1.389 (12) |
| C9—O7 | 1.272 (4) | C36—H36A | 0.9300 |
| C9—C10 | 1.485 (4) | C37—N8 | 1.333 (9) |
| C10—C11 | 1.392 (4) | C37—H37A | 0.9300 |

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|---|---|---|---|
| C10—C15 | 1.397 (4) | C38—N8 | 1.346 (6) |
| C11—C12 | 1.392 (5) | C38—C39 | 1.454 (6) |
| C11—H11A | 0.9300 | C39—C40 | 1.396 (7) |
| C12—O8 | 1.365 (4) | C39—C43 | 1.400 (5) |
| C12—C13 | 1.383 (5) | C40—C41 | 1.375 (7) |
| C13—C14 | 1.394 (5) | C40—H40A | 0.9300 |
| C13—H13A | 0.9300 | C41—C42 | 1.376 (6) |
| C14—C15 | 1.383 (4) | C41—H41A | 0.9300 |
| C14—C16 | 1.503 (4) | C42—N6 | 1.335 (5) |
| C15—H15A | 0.9300 | C42—H42A | 0.9300 |
| C16—O10 | 1.237 (4) | C43—N6 | 1.348 (4) |
| C16—O9 | 1.266 (4) | C43—C44 | 1.455 (5) |
| C16—Cd2$^{ii}$ | 2.685 (3) | C44—N5 | 1.339 (5) |
| C17—N1 | 1.320 (5) | O3—H3B | 0.8200 |
| C17—C18 | 1.392 (6) | O4—Cd1$^{i}$ | 2.360 (2) |
| C17—H17A | 0.9300 | O5—Cd1$^{i}$ | 2.384 (3) |
| C18—C19 | 1.372 (7) | O8—H8A | 0.8200 |
| C18—H18A | 0.9300 | O9—Cd2$^{ii}$ | 2.332 (2) |
| C19—C20 | 1.400 (6) | O10—Cd2$^{ii}$ | 2.362 (3) |
| C19—H19A | 0.9300 | O1W—H1WA | 0.8500 |
| C20—C30 | 1.396 (5) | O1W—H1WB | 0.8500 |
| C20—C21 | 1.457 (6) | O2W—H2WA | 0.8500 |
| C21—N3 | 1.354 (6) | O2W—H2WB | 0.8499 |

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| O7—Cd1—O1 | 92.68 (10) | C20—C19—H19A | 120.1 |
| O7—Cd1—N2 | 170.68 (10) | C30—C20—C19 | 117.5 (4) |
| O1—Cd1—N2 | 89.39 (10) | C30—C20—C21 | 119.9 (4) |
| O7—Cd1—O4$^{i}$ | 89.95 (10) | C19—C20—C21 | 122.5 (4) |
| O1—Cd1—O4$^{i}$ | 94.29 (9) | N3—C21—C24 | 122.4 (4) |
| N2—Cd1—O4$^{i}$ | 98.96 (10) | N3—C21—C20 | 117.7 (5) |
| O7—Cd1—N1 | 101.48 (11) | C24—C21—C20 | 119.9 (4) |
| O1—Cd1—N1 | 127.16 (9) | N3—C22—C23 | 122.1 (5) |
| N2—Cd1—N1 | 70.20 (10) | N3—C22—H22A | 118.9 |
| O4$^{i}$—Cd1—N1 | 135.72 (9) | C23—C22—H22A | 118.9 |
| O7—Cd1—O5$^{i}$ | 92.96 (11) | N4—C23—C22 | 123.9 (5) |
| O1—Cd1—O5$^{i}$ | 148.77 (9) | N4—C23—H23A | 118.0 |
| N2—Cd1—O5$^{i}$ | 89.96 (11) | C22—C23—H23A | 118.0 |
| O4$^{i}$—Cd1—O5$^{i}$ | 55.03 (9) | N4—C24—C21 | 121.5 (4) |
| N1—Cd1—O5$^{i}$ | 81.52 (9) | N4—C24—C25 | 118.2 (5) |
| O7—Cd1—C8$^{i}$ | 90.03 (10) | C21—C24—C25 | 120.3 (4) |
| O1—Cd1—C8$^{i}$ | 122.03 (10) | C29—C25—C26 | 117.2 (4) |
| N2—Cd1—C8$^{i}$ | 96.58 (11) | C29—C25—C24 | 119.7 (4) |
| O4$^{i}$—Cd1—C8$^{i}$ | 27.78 (9) | C26—C25—C24 | 123.0 (4) |
| N1—Cd1—C8$^{i}$ | 108.73 (10) | C27—C26—C25 | 119.7 (4) |
| O5$^{i}$—Cd1—C8$^{i}$ | 27.34 (10) | C27—C26—H26A | 120.1 |
| O2—Cd2—O6 | 89.39 (10) | C25—C26—H26A | 120.1 |
| O2—Cd2—N5 | 160.40 (10) | C26—C27—C28 | 119.4 (4) |
| O6—Cd2—N5 | 81.94 (10) | C26—C27—H27A | 120.3 |
| O2—Cd2—O9$^{ii}$ | 94.61 (10) | C28—C27—H27A | 120.3 |

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| O6—Cd2—O9$^{ii}$ | 98.31 (9) | N2—C28—C27 | 121.9 (4) |
| N5—Cd2—O9$^{ii}$ | 103.99 (10) | N2—C28—H28A | 119.1 |
| O2—Cd2—N6 | 97.96 (11) | C27—C28—H28A | 119.1 |
| O6—Cd2—N6 | 116.05 (10) | N2—C29—C25 | 122.7 (3) |
| N5—Cd2—N6 | 70.66 (10) | N2—C29—C30 | 117.1 (3) |
| O9$^{ii}$—Cd2—N6 | 143.34 (10) | C25—C29—C30 | 120.2 (3) |
| O2—Cd2—O10$^{ii}$ | 96.45 (11) | N1—C30—C20 | 122.3 (3) |
| O6—Cd2—O10$^{ii}$ | 153.41 (9) | N1—C30—C29 | 117.8 (3) |
| N5—Cd2—O10$^{ii}$ | 99.14 (11) | C20—C30—C29 | 119.9 (3) |
| O9$^{ii}$—Cd2—O10$^{ii}$ | 55.45 (9) | N5—C31—C32 | 121.7 (5) |
| N6—Cd2—O10$^{ii}$ | 88.88 (9) | N5—C31—H31A | 119.1 |
| O2—Cd2—C16$^{ii}$ | 94.70 (10) | C32—C31—H31A | 119.1 |
| O6—Cd2—C16$^{ii}$ | 126.42 (10) | C33—C32—C31 | 119.5 (5) |
| N5—Cd2—C16$^{ii}$ | 104.61 (10) | C33—C32—H32A | 120.3 |
| O9$^{ii}$—Cd2—C16$^{ii}$ | 28.12 (9) | C31—C32—H32A | 120.3 |
| N6—Cd2—C16$^{ii}$ | 116.16 (10) | C32—C33—C34 | 119.9 (4) |
| O10$^{ii}$—Cd2—C16$^{ii}$ | 27.42 (9) | C32—C33—H33A | 120.1 |
| O1—C1—O2 | 124.3 (3) | C34—C33—H33A | 120.1 |
| O1—C1—C2 | 120.1 (3) | C33—C34—C44 | 117.0 (4) |
| O2—C1—C2 | 115.6 (3) | C33—C34—C35 | 123.8 (4) |
| C7—C2—C3 | 120.5 (3) | C44—C34—C35 | 119.1 (4) |
| C7—C2—C1 | 119.4 (3) | N7—C35—C38 | 120.8 (5) |
| C3—C2—C1 | 120.0 (3) | N7—C35—C34 | 118.1 (6) |
| C2—C3—C4 | 119.2 (3) | C38—C35—C34 | 121.1 (4) |
| C2—C3—H3A | 120.4 | N7—C36—C37 | 123.5 (6) |
| C4—C3—H3A | 120.4 | N7—C36—H36A | 118.3 |
| C5—C4—C3 | 120.1 (3) | C37—C36—H36A | 118.3 |
| C5—C4—C8 | 119.4 (3) | N8—C37—C36 | 121.6 (6) |
| C3—C4—C8 | 120.5 (3) | N8—C37—H37A | 119.2 |
| C6—C5—C4 | 120.3 (3) | C36—C37—H37A | 119.2 |
| C6—C5—H5A | 119.9 | N8—C38—C35 | 122.7 (5) |
| C4—C5—H5A | 119.9 | N8—C38—C39 | 117.3 (5) |
| O3—C6—C5 | 118.4 (3) | C35—C38—C39 | 120.0 (4) |
| O3—C6—C7 | 121.6 (3) | C40—C39—C43 | 117.4 (4) |
| C5—C6—C7 | 120.0 (3) | C40—C39—C38 | 123.2 (4) |
| C6—C7—C2 | 119.9 (3) | C43—C39—C38 | 119.3 (4) |
| C6—C7—H7A | 120.0 | C41—C40—C39 | 119.7 (4) |
| C2—C7—H7A | 120.0 | C41—C40—H40A | 120.2 |
| O5—C8—O4 | 121.7 (3) | C39—C40—H40A | 120.2 |
| O5—C8—C4 | 119.4 (3) | C40—C41—C42 | 119.5 (4) |
| O4—C8—C4 | 118.9 (3) | C40—C41—H41A | 120.2 |
| O5—C8—Cd1$^{i}$ | 61.56 (18) | C42—C41—H41A | 120.2 |
| O4—C8—Cd1$^{i}$ | 60.48 (17) | N6—C42—C41 | 121.9 (4) |
| C4—C8—Cd1$^{i}$ | 174.5 (3) | N6—C42—H42A | 119.1 |
| O6—C9—O7 | 122.8 (3) | C41—C42—H42A | 119.1 |
| O6—C9—C10 | 120.6 (3) | N6—C43—C39 | 122.0 (3) |
| O7—C9—C10 | 116.6 (3) | N6—C43—C44 | 117.4 (3) |
| C11—C10—C15 | 120.3 (3) | C39—C43—C44 | 120.6 (3) |
| C11—C10—C9 | 118.7 (3) | N5—C44—C34 | 122.4 (4) |

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|---|---|---|---|
| C15—C10—C9 | 120.8 (3) | N5—C44—C43 | 117.7 (3) |
| C12—C11—C10 | 120.0 (3) | C34—C44—C43 | 119.9 (4) |
| C12—C11—H11A | 120.0 | C17—N1—C30 | 118.9 (3) |
| C10—C11—H11A | 120.0 | C17—N1—Cd1 | 124.1 (2) |
| O8—C12—C13 | 118.9 (3) | C30—N1—Cd1 | 115.3 (2) |
| O8—C12—C11 | 121.4 (3) | C28—N2—C29 | 119.1 (3) |
| C13—C12—C11 | 119.7 (3) | C28—N2—Cd1 | 123.2 (3) |
| C12—C13—C14 | 120.2 (3) | C29—N2—Cd1 | 116.6 (2) |
| C12—C13—H13A | 119.9 | C22—N3—C21 | 115.1 (6) |
| C14—C13—H13A | 119.9 | C23—N4—C24 | 115.0 (6) |
| C15—C14—C13 | 120.6 (3) | C31—N5—C44 | 119.5 (3) |
| C15—C14—C16 | 120.3 (3) | C31—N5—Cd2 | 123.0 (3) |
| C13—C14—C16 | 119.1 (3) | C44—N5—Cd2 | 117.4 (2) |
| C14—C15—C10 | 119.1 (3) | C42—N6—C43 | 119.3 (3) |
| C14—C15—H15A | 120.4 | C42—N6—Cd2 | 124.0 (2) |
| C10—C15—H15A | 120.4 | C43—N6—Cd2 | 116.7 (2) |
| O10—C16—O9 | 121.5 (3) | C36—N7—C35 | 115.4 (7) |
| O10—C16—C14 | 119.6 (3) | C37—N8—C38 | 116.0 (7) |
| O9—C16—C14 | 118.9 (3) | C1—O1—Cd1 | 139.9 (2) |
| O10—C16—Cd2$^{ii}$ | 61.58 (18) | C1—O2—Cd2 | 116.7 (2) |
| O9—C16—Cd2$^{ii}$ | 60.23 (17) | C6—O3—H3B | 109.5 |
| C14—C16—Cd2$^{ii}$ | 175.5 (2) | C8—O4—Cd1$^{i}$ | 91.74 (19) |
| N1—C17—C18 | 122.7 (4) | C8—O5—Cd1$^{i}$ | 91.1 (2) |
| N1—C17—H17A | 118.6 | C9—O6—Cd2 | 142.2 (2) |
| C18—C17—H17A | 118.6 | C9—O7—Cd1 | 112.1 (2) |
| C19—C18—C17 | 118.8 (4) | C12—O8—H8A | 109.5 |
| C19—C18—H18A | 120.6 | C16—O9—Cd2$^{ii}$ | 91.65 (19) |
| C17—C18—H18A | 120.6 | C16—O10—Cd2$^{ii}$ | 91.0 (2) |
| C18—C19—C20 | 119.7 (4) | H1WA—O1W—H1WB | 120.0 |
| C18—C19—H19A | 120.1 | H2WA—O2W—H2WB | 120.0 |

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| O1—C1—C2—C7 | 154.7 (3) | O1—Cd1—N1—C17 | −107.3 (3) |
| O2—C1—C2—C7 | −26.3 (5) | N2—Cd1—N1—C17 | 179.4 (3) |
| O1—C1—C2—C3 | −29.3 (5) | O4$^{i}$—Cd1—N1—C17 | 97.0 (3) |
| O2—C1—C2—C3 | 149.8 (3) | O5$^{i}$—Cd1—N1—C17 | 86.3 (3) |
| C7—C2—C3—C4 | 2.3 (5) | C8$^{i}$—Cd1—N1—C17 | 89.0 (3) |
| C1—C2—C3—C4 | −173.8 (3) | O7—Cd1—N1—C30 | −169.8 (2) |
| C2—C3—C4—C5 | −2.6 (5) | O1—Cd1—N1—C30 | 87.8 (3) |
| C2—C3—C4—C8 | 177.6 (3) | N2—Cd1—N1—C30 | 14.5 (2) |
| C3—C4—C5—C6 | 1.4 (5) | O4$^{i}$—Cd1—N1—C30 | −67.9 (3) |
| C8—C4—C5—C6 | −178.7 (3) | O5$^{i}$—Cd1—N1—C30 | −78.5 (2) |
| C4—C5—C6—O3 | 179.7 (3) | C8$^{i}$—Cd1—N1—C30 | −75.8 (2) |
| C4—C5—C6—C7 | 0.1 (6) | C27—C28—N2—C29 | 0.5 (7) |
| O3—C6—C7—C2 | 179.9 (3) | C27—C28—N2—Cd1 | 168.1 (4) |
| C5—C6—C7—C2 | −0.5 (6) | C25—C29—N2—C28 | 1.6 (5) |
| C3—C2—C7—C6 | −0.7 (5) | C30—C29—N2—C28 | −178.9 (3) |
| C1—C2—C7—C6 | 175.3 (3) | C25—C29—N2—Cd1 | −166.8 (3) |
| C5—C4—C8—O5 | −17.3 (5) | C30—C29—N2—Cd1 | 12.7 (4) |
| C3—C4—C8—O5 | 162.5 (3) | O7—Cd1—N2—C28 | 150.5 (6) |

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| C5—C4—C8—O4 | 162.5 (3) | O1—Cd1—N2—C28 | 47.7 (3) |
| C3—C4—C8—O4 | −17.7 (5) | O4$^{i}$—Cd1—N2—C28 | −46.6 (3) |
| C5—C4—C8—Cd1$^{i}$ | −116 (2) | N1—Cd1—N2—C28 | 177.9 (3) |
| C3—C4—C8—Cd1$^{i}$ | 64 (3) | O5$^{i}$—Cd1—N2—C28 | −101.1 (3) |
| O6—C9—C10—C11 | 156.7 (3) | C8$^{i}$—Cd1—N2—C28 | −74.5 (3) |
| O7—C9—C10—C11 | −24.2 (5) | O7—Cd1—N2—C29 | −41.6 (8) |
| O6—C9—C10—C15 | −27.4 (5) | O1—Cd1—N2—C29 | −144.5 (3) |
| O7—C9—C10—C15 | 151.7 (3) | O4$^{i}$—Cd1—N2—C29 | 121.3 (2) |
| C15—C10—C11—C12 | −0.3 (5) | N1—Cd1—N2—C29 | −14.3 (2) |
| C9—C10—C11—C12 | 175.6 (3) | O5$^{i}$—Cd1—N2—C29 | 66.7 (2) |
| C10—C11—C12—O8 | −178.8 (3) | C8$^{i}$—Cd1—N2—C29 | 93.3 (3) |
| C10—C11—C12—C13 | −1.2 (6) | C23—C22—N3—C21 | 0.8 (9) |
| O8—C12—C13—C14 | 178.6 (3) | C24—C21—N3—C22 | −1.6 (7) |
| C11—C12—C13—C14 | 1.0 (6) | C20—C21—N3—C22 | 179.9 (5) |
| C12—C13—C14—C15 | 0.7 (5) | C22—C23—N4—C24 | 0.4 (10) |
| C12—C13—C14—C16 | 180.0 (3) | C21—C24—N4—C23 | −1.2 (8) |
| C13—C14—C15—C10 | −2.3 (5) | C25—C24—N4—C23 | 178.2 (5) |
| C16—C14—C15—C10 | 178.5 (3) | C32—C31—N5—C44 | −0.3 (6) |
| C11—C10—C15—C14 | 2.0 (5) | C32—C31—N5—Cd2 | −176.9 (4) |
| C9—C10—C15—C14 | −173.8 (3) | C34—C44—N5—C31 | −0.7 (5) |
| C15—C14—C16—O10 | 162.0 (3) | C43—C44—N5—C31 | 179.3 (3) |
| C13—C14—C16—O10 | −17.3 (5) | C34—C44—N5—Cd2 | 176.1 (3) |
| C15—C14—C16—O9 | −19.1 (5) | C43—C44—N5—Cd2 | −4.0 (4) |
| C13—C14—C16—O9 | 161.7 (3) | O2—Cd2—N5—C31 | 123.5 (4) |
| C15—C14—C16—Cd2$^{ii}$ | 58 (3) | O6—Cd2—N5—C31 | 59.0 (3) |
| C13—C14—C16—Cd2$^{ii}$ | −121 (3) | O9$^{ii}$—Cd2—N5—C31 | −37.7 (3) |
| N1—C17—C18—C19 | 0.7 (7) | N6—Cd2—N5—C31 | −179.7 (3) |
| C17—C18—C19—C20 | 0.7 (7) | O10$^{ii}$—Cd2—N5—C31 | −94.2 (3) |
| C18—C19—C20—C30 | −1.1 (7) | C16$^{ii}$—Cd2—N5—C31 | −66.7 (3) |
| C18—C19—C20—C21 | 178.4 (4) | O2—Cd2—N5—C44 | −53.1 (4) |
| C30—C20—C21—N3 | 176.8 (4) | O6—Cd2—N5—C44 | −117.7 (3) |
| C19—C20—C21—N3 | −2.7 (6) | O9$^{ii}$—Cd2—N5—C44 | 145.7 (2) |
| C30—C20—C21—C24 | −1.8 (6) | N6—Cd2—N5—C44 | 3.6 (2) |
| C19—C20—C21—C24 | 178.8 (4) | O10$^{ii}$—Cd2—N5—C44 | 89.2 (2) |
| N3—C22—C23—N4 | −0.2 (12) | C16$^{ii}$—Cd2—N5—C44 | 116.7 (2) |
| N3—C21—C24—N4 | 1.9 (7) | C41—C42—N6—C43 | 0.3 (6) |
| C20—C21—C24—N4 | −179.6 (4) | C41—C42—N6—Cd2 | −179.8 (3) |
| N3—C21—C24—C25 | −177.5 (4) | C39—C43—N6—C42 | 1.8 (5) |
| C20—C21—C24—C25 | 1.0 (6) | C44—C43—N6—C42 | −178.1 (3) |
| N4—C24—C25—C29 | −179.1 (4) | C39—C43—N6—Cd2 | −178.0 (3) |
| C21—C24—C25—C29 | 0.3 (6) | C44—C43—N6—Cd2 | 2.0 (4) |
| N4—C24—C25—C26 | 1.8 (7) | O2—Cd2—N6—C42 | −19.2 (3) |
| C21—C24—C25—C26 | −178.8 (5) | O6—Cd2—N6—C42 | −112.5 (3) |
| C29—C25—C26—C27 | 0.6 (8) | N5—Cd2—N6—C42 | 177.2 (3) |
| C24—C25—C26—C27 | 179.7 (5) | O9$^{ii}$—Cd2—N6—C42 | 89.6 (3) |
| C25—C26—C27—C28 | 1.3 (9) | O10$^{ii}$—Cd2—N6—C42 | 77.1 (3) |
| C26—C27—C28—N2 | −1.9 (9) | C16$^{ii}$—Cd2—N6—C42 | 80.0 (3) |
| C26—C25—C29—N2 | −2.1 (6) | O2—Cd2—N6—C43 | 160.6 (2) |
| C24—C25—C29—N2 | 178.8 (4) | O6—Cd2—N6—C43 | 67.4 (3) |

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| C26—C25—C29—C30 | 178.3 (4) | N5—Cd2—N6—C43 | −2.9 (2) |
| C24—C25—C29—C30 | −0.8 (5) | O9$^{ii}$—Cd2—N6—C43 | −90.5 (3) |
| C19—C20—C30—N1 | 0.3 (6) | O10$^{ii}$—Cd2—N6—C43 | −103.0 (2) |
| C21—C20—C30—N1 | −179.2 (3) | C16$^{ii}$—Cd2—N6—C43 | −100.1 (2) |
| C19—C20—C30—C29 | −179.2 (4) | C37—C36—N7—C35 | 0.8 (10) |
| C21—C20—C30—C29 | 1.2 (5) | C38—C35—N7—C36 | −1.9 (7) |
| N2—C29—C30—N1 | 0.9 (5) | C34—C35—N7—C36 | 178.5 (5) |
| C25—C29—C30—N1 | −179.5 (3) | C36—C37—N8—C38 | −1.4 (10) |
| N2—C29—C30—C20 | −179.6 (3) | C35—C38—N8—C37 | 0.3 (8) |
| C25—C29—C30—C20 | 0.0 (5) | C39—C38—N8—C37 | −179.4 (5) |
| N5—C31—C32—C33 | 1.1 (8) | O2—C1—O1—Cd1 | −83.6 (5) |
| C31—C32—C33—C34 | −0.9 (8) | C2—C1—O1—Cd1 | 95.4 (4) |
| C32—C33—C34—C44 | −0.1 (7) | O7—Cd1—O1—C1 | −1.5 (4) |
| C32—C33—C34—C35 | −179.0 (5) | N2—Cd1—O1—C1 | 169.4 (4) |
| C33—C34—C35—N7 | −2.4 (7) | O4$^{i}$—Cd1—O1—C1 | −91.7 (4) |
| C44—C34—C35—N7 | 178.7 (4) | N1—Cd1—O1—C1 | 105.0 (4) |
| C33—C34—C35—C38 | 177.9 (5) | O5$^{i}$—Cd1—O1—C1 | −101.7 (4) |
| C44—C34—C35—C38 | −1.0 (6) | C8$^{i}$—Cd1—O1—C1 | −93.3 (4) |
| N7—C36—C37—N8 | 0.9 (12) | O1—C1—O2—Cd2 | 7.4 (5) |
| N7—C35—C38—N8 | 1.4 (7) | C2—C1—O2—Cd2 | −171.6 (2) |
| C34—C35—C38—N8 | −178.9 (4) | O6—Cd2—O2—C1 | 61.2 (3) |
| N7—C35—C38—C39 | −178.9 (4) | N5—Cd2—O2—C1 | −2.2 (5) |
| C34—C35—C38—C39 | 0.8 (6) | O9$^{ii}$—Cd2—O2—C1 | 159.5 (3) |
| N8—C38—C39—C40 | 1.0 (6) | N6—Cd2—O2—C1 | −55.1 (3) |
| C35—C38—C39—C40 | −178.8 (4) | O10$^{ii}$—Cd2—O2—C1 | −144.8 (3) |
| N8—C38—C39—C43 | −179.8 (4) | C16$^{ii}$—Cd2—O2—C1 | −172.3 (3) |
| C35—C38—C39—C43 | 0.4 (6) | O5—C8—O4—Cd1$^{i}$ | −6.4 (4) |
| C43—C39—C40—C41 | 0.3 (7) | C4—C8—O4—Cd1$^{i}$ | 173.7 (3) |
| C38—C39—C40—C41 | 179.5 (4) | O4—C8—O5—Cd1$^{i}$ | 6.4 (4) |
| C39—C40—C41—C42 | 1.7 (7) | C4—C8—O5—Cd1$^{i}$ | −173.8 (3) |
| C40—C41—C42—N6 | −2.1 (7) | O7—C9—O6—Cd2 | −93.2 (5) |
| C40—C39—C43—N6 | −2.1 (5) | C10—C9—O6—Cd2 | 85.9 (5) |
| C38—C39—C43—N6 | 178.6 (3) | O2—Cd2—O6—C9 | 10.2 (4) |
| C40—C39—C43—C44 | 177.8 (4) | N5—Cd2—O6—C9 | 172.6 (4) |
| C38—C39—C43—C44 | −1.5 (5) | O9$^{ii}$—Cd2—O6—C9 | −84.4 (4) |
| C33—C34—C44—N5 | 0.9 (6) | N6—Cd2—O6—C9 | 108.8 (4) |
| C35—C34—C44—N5 | 179.9 (3) | O10$^{ii}$—Cd2—O6—C9 | −93.1 (5) |
| C33—C34—C44—C43 | −179.0 (4) | C16$^{ii}$—Cd2—O6—C9 | −85.2 (4) |
| C35—C34—C44—C43 | −0.1 (5) | O6—C9—O7—Cd1 | 7.5 (4) |
| N6—C43—C44—N5 | 1.3 (5) | C10—C9—O7—Cd1 | −171.6 (2) |
| C39—C43—C44—N5 | −178.6 (3) | O1—Cd1—O7—C9 | 64.0 (3) |
| N6—C43—C44—C34 | −178.8 (3) | N2—Cd1—O7—C9 | −38.6 (8) |
| C39—C43—C44—C34 | 1.3 (5) | O4$^{i}$—Cd1—O7—C9 | 158.3 (3) |
| C18—C17—N1—C30 | −1.5 (6) | N1—Cd1—O7—C9 | −64.8 (3) |
| C18—C17—N1—Cd1 | −165.9 (3) | O5$^{i}$—Cd1—O7—C9 | −146.8 (3) |
| C20—C30—N1—C17 | 1.0 (5) | C8$^{i}$—Cd1—O7—C9 | −174.0 (3) |
| C29—C30—N1—C17 | −179.4 (3) | O10—C16—O9—Cd2$^{ii}$ | −6.2 (4) |
| C20—C30—N1—Cd1 | 166.7 (3) | C14—C16—O9—Cd2$^{ii}$ | 174.9 (3) |

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| C29—C30—N1—Cd1 | −13.8 (4) | O9—C16—O10—Cd2$^{ii}$ | 6.1 (4) |
| O7—Cd1—N1—C17 | −5.0 (3) | C14—C16—O10—Cd2$^{ii}$ | −175.0 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3*B*···O2*W*$^{iii}$ | 0.82 | 1.84 | 2.659 (4) | 177 |
| O8—H8*A*···O1*W*$^{iv}$ | 0.82 | 1.85 | 2.672 (4) | 177 |
| O1*W*—H1*WA*···O9$^{v}$ | 0.85 | 2.14 | 2.912 (4) | 150 |
| O1*W*—H1*WB*···O2$^{v}$ | 0.85 | 2.27 | 2.963 (4) | 138 |
| O2*W*—H2*WA*···O4$^{vi}$ | 0.85 | 2.28 | 2.880 (4) | 127 |
| O2*W*—H2*WB*···O7$^{vi}$ | 0.85 | 2.33 | 2.955 (4) | 131 |

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