Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Di-$\mu$-acetato-$\kappa^4O$:$O$-bis{(acetato-$\kappa^2O,O'$)bis[3-(1*H*-imidazol-1-yl-$\kappa N^3$)-1-phenylpropan-1-one]cadmium} tetrahydrate

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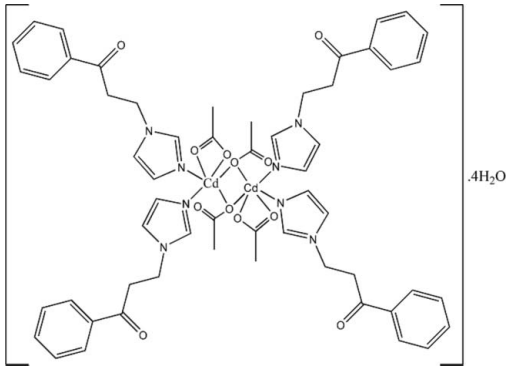
Received 10 November 2011; accepted 22 November 2011

Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.031; $wR$ factor = 0.077; data-to-parameter ratio = 18.3.

In the molecular structure of the title neutral binuclear complex, $[Cd_2(C_2H_3O_2)_4(C_{12}H_{12}N_2O)_4]\cdot 4H_2O$, each $Cd^{II}$ atom is six-coordinated and exhibits a distorted octahedral geometry. Three O atoms from two acetate ions and one monodentate 3-(1*H*-imidazol-1-yl-$\kappa N^3$)-1-phenylpropan-1-one (*L*) ligand form the equatorial plane, while the bridging-O atom forming the longer Cd—O distance,and the N atom of the second *L* ligand, forming the longer Cd—N distance, occupy axial positions with an N—Cd—O angle of 170.77 (7)°. Intermolecular O—H···O hydrogen bonds exist between the lattice water molecules and the acetate ions of adjacent molecules, resulting in a two-dimensional supramolecular structure.

## Related literature

For reviews on the generation of supramolecular structures based on coordination complexes, see: Barnett & Champness (2003); Roesky & Andruh (2003); Zaworotko (2001).




## Experimental

### Crystal data

$[Cd_2(C_2H_3O_2)_4(C_{12}H_{12}N_2O)_4]\cdot 4H_2O$
$M_r$ = 1333.98
Monoclinic, $P2_1/c$
$a$ = 18.818 (3) Å
$b$ = 10.6490 (17) Å
$c$ = 15.864 (3) Å
$\beta$ = 112.036 (2)°
$V$ = 2946.8 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.80 mm$^{-1}$
$T$ = 296 K
0.28 × 0.22 × 0.20 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.808, $T_{max}$ = 0.857
17422 measured reflections
6806 independent reflections
4666 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.077
$S$ = 1.00
6806 reflections
372 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.46 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cd1—O5$^{i}$ | 2.2331 (18) | Cd1—O3 | 2.354 (2) |
| Cd1—N1 | 2.238 (2) | Cd1—O4 | 2.446 (2) |
| Cd1—N3 | 2.349 (2) | Cd1—O5 | 2.5855 (18) |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O7—H7$A$···O3$^{ii}$ | 0.85 | 2.11 | 2.949 (3) | 169 |
| O7—H7$B$···O4$^{iii}$ | 0.85 | 1.99 | 2.829 (3) | 171 |
| O8—H8$B$···O6$^{iii}$ | 0.85 | 2.03 | 2.838 (3) | 159 |
| O8—H8$A$···O7$^{iv}$ | 0.85 | 1.97 | 2.818 (3) | 174 |

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2039).

## References

Barnett, S. A. & Champness, N. R. (2003). *Coord. Chem. Rev.* **246**, 145–168.
Brandenburg, K. & Berndt, M. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2003). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Roesky, H. W. & Andruh, M. (2003). *Coord. Chem. Rev.* **236**, 91–119.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zaworotko, M. J. (2001). *Chem. Commun.* pp. 1–9.

# supporting information

*Acta Cryst.* (2011). E**67**, m1884 [https://doi.org/10.1107/S1600536811050021]

## Di-$\mu$-acetato-$\kappa^4O$:$O$-bis{(acetato-$\kappa^2O,O'$)bis[3-(1*H*-imidazol-1-yl-$\kappa N^3$)-1-phenylpropan-1-one]cadmium} tetrahydrate

**Jian-Hua Guo**

### S1. Comment

Neutral organic ligands containing rigid or flexible spacers, such as 4,4′-bipyridine, 1,2-bis(4′-pyridyl)ethane, 1,2-bis(4-pyridyl)propane and many others, have been used to generate a rich variety of metal-organic architectures with different metal ions by various reaction procedures (Barnett & Champness, 2003; Zaworotko, 2001; Roesky & Andruh, 2003). In our recent research, we have initiated a synthetic approach employing the ligand 3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one (*L*), which consists of a propanone unit substituted with an imidazole and a phenyl group, in reaction with different metal ions to construct new functional frameworks. To explore this series, we synthesized the title compound, (I), a new $Cd^{II}$ complex based on *L*. In the molecular structure of (I) (Fig. 1) each $Cd^{II}$ atom is six-coordinated and exhibits a distorted octahedral geometry. Three O atoms from two acetate ions and one monodentate *L* ligand form the equatorial plane while one O atom from one acetate ion and the other monodentate *L* ligand occupy axial positions with an N3—Cd1—O5 angle of 170.77 (7)°. Atoms O5 and O5A of one pair of acetate ions serve to bridge the $Cd^{II}$ centers in the centrosymmetric binuclear units. The mean planes of the imidazole and phenyl rings in the two unique ligands are nearly perpendicular to one another with the angles between these planes being 78.6 (1)° and 76.2 (1)°, respectively. Analysis of the crystal packing indicates that intermolecular O—H···O hydrogen bonds involving the lattice water molecules and both types of actate ions extend the binuclear units to produce a 2-D supramolecular framework structure, as shown in Fig. 2.

### S2. Experimental

$Cd(OAc)_2.2H_2O$ (26.7 mg, 0.1 mmol) and 3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one (22.2 mg, 0.1 mmol) were mixed in a $CH_3CN/H_2O$ (20 ml, 1:1 *v*/*v*) solution with vigorous stirring for *ca* 30 min. The resulting solution was filtered and left to stand at room temperature. Colorless block crystals of (I) suitable for X-ray analysis were obtained in 75% yield by slow evaporation of the solvent over a period of 1 week. Analysis, calculated for $CdC_{28}H_{34}N_4O_8$: C 50.42, H 5.14, N 8.40; found: C 50.45, H 5.03, N 8.32.

### S3. Refinement

Although all H atoms were visible in difference maps, they were placed in geometrically calculated positions, with C—H and O—H distances in the range 0.93–0.97Å and 0.85 Å, respectively, and included in the final refinement in the riding model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(C) for aromatic and methylene H atoms. and $U_{iso}$(H) = 1.5$U_{eq}$(C or O) for methyl and $H_2O$ H atoms

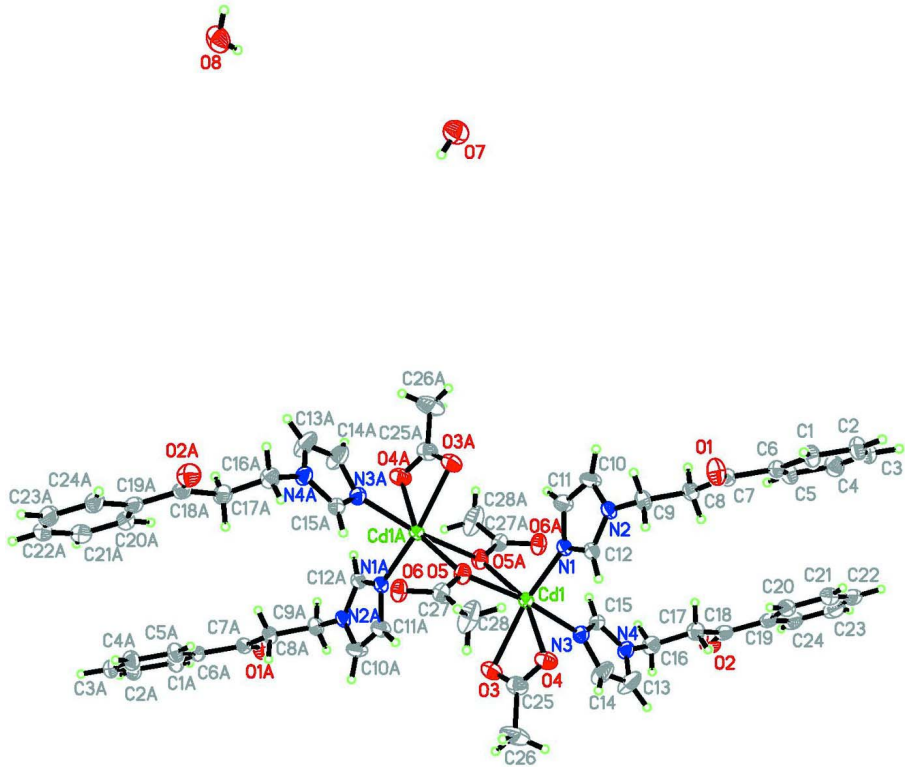



**Figure 1**

The molecular structure of (I) using 30% probability ellipsoids (Symmetry transformation used to generate equivalent atoms: -x+1,-y+2,-z+2).

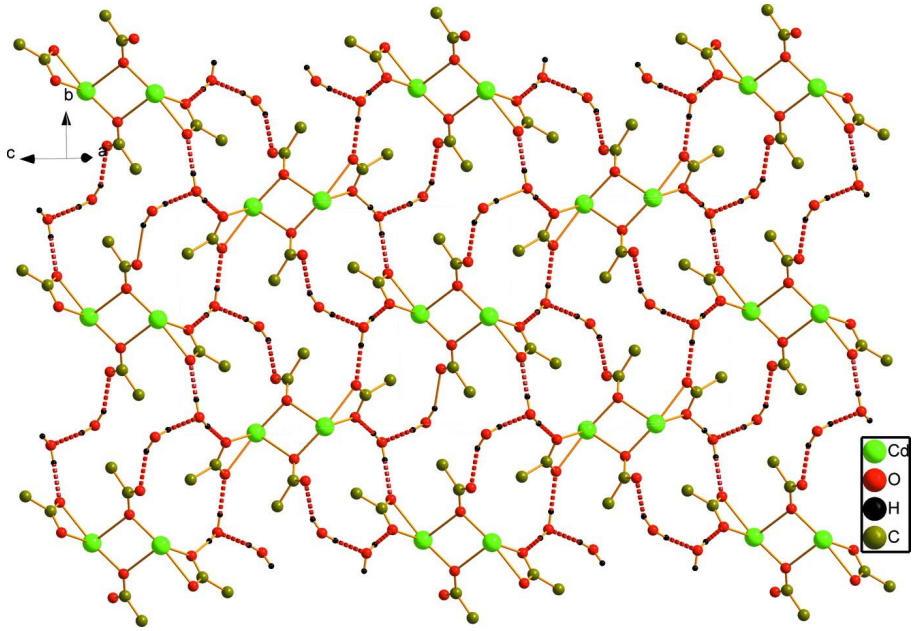



**Figure 2**

The 2-D supramolecular framework structure of compound, showing O—H···O hydrogen bonds as red dashed lines (the *L* ligands have been removed for clarity).

**Di-$\mu$-acetato-$\kappa^4O$:$O$-bis{(acetato- $\kappa^2O,O'$)bis[3-(1*H*-imidazol-1-yl- $\kappa N^3$)-1-phenylpropan-1-one]cadmium} tetrahydrate**

*Crystal data*

$[Cd_2(C_2H_3O_2)_4(C_{12}H_{12}N_2O)_4]\cdot 4H_2O$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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$b = 10.6490$ (17) Å
$c = 15.864$ (3) Å
$\beta = 112.036$ (2)°
$V = 2946.8$ (8) Å$^3$
$Z = 2$
$F(000) = 1368$
$D_x = 1.503$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4777 reflections
$\theta = 2.6$–25.4°
$\mu = 0.80$ mm$^{-1}$
$T = 296$ K
Block, colorless
0.28 × 0.22 × 0.20 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.808$, $T_{max} = 0.857$
17422 measured reflections
6806 independent reflections
4666 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.2°$
$h = -24\rightarrow24$
$k = -13\rightarrow7$
$l = -19\rightarrow20$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.077$
$S = 1.00$
6806 reflections
372 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 1.0868P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.53$ e Å$^{-3}$
$\Delta\rho_{min} = -0.46$ 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 | 0.421249 (10) | 0.990415 (18) | 1.052021 (12) | 0.03958 (7) |
| O1 | 0.08650 (12) | 0.52281 (17) | 0.69389 (16) | 0.0617 (6) |
| O2 | 0.09479 (14) | 1.4665 (2) | 1.14769 (16) | 0.0664 (6) |

| | | | | |
|---|---|---|---|---|
| O3 | 0.50729 (12) | 0.9464 (2) | 1.20070 (14) | 0.0602 (5) |
| O4 | 0.41427 (12) | 0.80882 (18) | 1.14306 (14) | 0.0577 (5) |
| O5 | 0.51810 (10) | 0.86982 (17) | 1.00202 (13) | 0.0477 (5) |
| O6 | 0.62749 (11) | 0.76847 (17) | 1.04134 (15) | 0.0548 (5) |
| O7 | 0.37028 (13) | 0.5542 (2) | 0.13904 (16) | 0.0776 (7) |
| H7A | 0.4013 | 0.5150 | 0.1847 | 0.116* |
| H7B | 0.3785 | 0.6323 | 0.1363 | 0.116* |
| O8 | 0.69937 (13) | 0.5343 (2) | 0.04085 (17) | 0.0788 (7) |
| H8A | 0.6793 | 0.5019 | −0.0118 | 0.118* |
| H8B | 0.6753 | 0.5955 | 0.0522 | 0.118* |
| N1 | 0.33866 (12) | 0.9077 (2) | 0.92267 (14) | 0.0397 (5) |
| N2 | 0.25575 (12) | 0.7856 (2) | 0.82184 (15) | 0.0411 (5) |
| N3 | 0.33891 (13) | 1.0771 (2) | 1.11710 (16) | 0.0458 (5) |
| N4 | 0.26263 (13) | 1.2047 (2) | 1.15386 (16) | 0.0478 (6) |
| C1 | −0.07134 (16) | 0.5507 (3) | 0.6383 (2) | 0.0521 (7) |
| H1 | −0.0525 | 0.4736 | 0.6285 | 0.062* |
| C2 | −0.14918 (18) | 0.5682 (3) | 0.6113 (2) | 0.0621 (9) |
| H2 | −0.1825 | 0.5029 | 0.5833 | 0.075* |
| C3 | −0.17788 (17) | 0.6812 (3) | 0.6253 (2) | 0.0575 (8) |
| H3 | −0.2305 | 0.6925 | 0.6070 | 0.069* |
| C4 | −0.12871 (17) | 0.7779 (3) | 0.6664 (2) | 0.0585 (8) |
| H4 | −0.1482 | 0.8548 | 0.6754 | 0.070* |
| C5 | −0.05019 (16) | 0.7610 (3) | 0.6943 (2) | 0.0506 (7) |
| H5 | −0.0171 | 0.8264 | 0.7228 | 0.061* |
| C6 | −0.02075 (15) | 0.6472 (2) | 0.68013 (18) | 0.0404 (6) |
| C7 | 0.06321 (15) | 0.6234 (2) | 0.70880 (18) | 0.0412 (6) |
| C8 | 0.11922 (14) | 0.7264 (2) | 0.75563 (18) | 0.0421 (6) |
| H8A′ | 0.1106 | 0.7533 | 0.8094 | 0.051* |
| H8B′ | 0.1104 | 0.7979 | 0.7151 | 0.051* |
| C9 | 0.20162 (15) | 0.6829 (2) | 0.7829 (2) | 0.0460 (7) |
| H9A | 0.2116 | 0.6157 | 0.8271 | 0.055* |
| H9B | 0.2092 | 0.6499 | 0.7299 | 0.055* |
| C10 | 0.27050 (18) | 0.8835 (3) | 0.77606 (19) | 0.0588 (8) |
| H10 | 0.2492 | 0.8969 | 0.7136 | 0.071* |
| C11 | 0.32162 (17) | 0.9573 (3) | 0.8380 (2) | 0.0535 (8) |
| H11 | 0.3423 | 1.0308 | 0.8253 | 0.064* |
| C12 | 0.29864 (15) | 0.8039 (3) | 0.91023 (18) | 0.0435 (6) |
| H12 | 0.2998 | 0.7497 | 0.9567 | 0.052* |
| C13 | 0.2737 (2) | 1.1008 (3) | 1.2069 (3) | 0.0884 (14) |
| H13 | 0.2532 | 1.0861 | 1.2511 | 0.106* |
| C14 | 0.3193 (2) | 1.0238 (3) | 1.1839 (3) | 0.0791 (12) |
| H14 | 0.3355 | 0.9452 | 1.2095 | 0.095* |
| C15 | 0.30280 (15) | 1.1856 (3) | 1.10107 (19) | 0.0456 (7) |
| H15 | 0.3050 | 1.2428 | 1.0578 | 0.055* |
| C16 | 0.21135 (17) | 1.3088 (3) | 1.1499 (2) | 0.0533 (7) |
| H16A | 0.2235 | 1.3793 | 1.1189 | 0.064* |
| H16B | 0.2189 | 1.3352 | 1.2112 | 0.064* |
| C17 | 0.12822 (16) | 1.2713 (3) | 1.1001 (2) | 0.0529 (7) |

| | | | | |
|---|---|---|---|---|
| H17A | 0.1193 | 1.2571 | 1.0366 | 0.063* |
| H17B | 0.1188 | 1.1928 | 1.1252 | 0.063* |
| C18 | 0.07216 (17) | 1.3690 (3) | 1.10664 (19) | 0.0496 (7) |
| C19 | −0.01133 (18) | 1.3416 (3) | 1.0617 (2) | 0.0528 (8) |
| C20 | −0.03927 (19) | 1.2307 (4) | 1.0159 (2) | 0.0643 (9) |
| H20 | −0.0052 | 1.1694 | 1.0127 | 0.077* |
| C21 | −0.1179 (2) | 1.2100 (4) | 0.9745 (2) | 0.0803 (11) |
| H21 | −0.1363 | 1.1349 | 0.9442 | 0.096* |
| C22 | −0.1684 (2) | 1.3016 (6) | 0.9789 (3) | 0.0948 (15) |
| H22 | −0.2209 | 1.2887 | 0.9508 | 0.114* |
| C23 | −0.1412 (3) | 1.4115 (5) | 1.0246 (3) | 0.0941 (15) |
| H23 | −0.1755 | 1.4725 | 1.0278 | 0.113* |
| C24 | −0.0635 (2) | 1.4325 (4) | 1.0659 (2) | 0.0701 (10) |
| H24 | −0.0456 | 1.5074 | 1.0967 | 0.084* |
| C25 | 0.4710 (2) | 0.8497 (3) | 1.2087 (2) | 0.0580 (8) |
| C26 | 0.4947 (2) | 0.7839 (4) | 1.2998 (2) | 0.0951 (13) |
| H26A | 0.4505 | 0.7716 | 1.3152 | 0.143* |
| H26B | 0.5316 | 0.8344 | 1.3456 | 0.143* |
| H26C | 0.5170 | 0.7040 | 1.2962 | 0.143* |
| C27 | 0.55988 (16) | 0.7733 (2) | 1.03291 (19) | 0.0414 (6) |
| C28 | 0.5239 (2) | 0.6615 (3) | 1.0586 (3) | 0.0913 (14) |
| H28A | 0.5395 | 0.5864 | 1.0368 | 0.137* |
| H28B | 0.4691 | 0.6690 | 1.0319 | 0.137* |
| H28C | 0.5402 | 0.6574 | 1.1236 | 0.137* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.03298 (11) | 0.04915 (12) | 0.03321 (10) | −0.00241 (9) | 0.00850 (8) | −0.00217 (9) |
| O1 | 0.0458 (12) | 0.0424 (11) | 0.0913 (17) | −0.0026 (9) | 0.0192 (12) | −0.0128 (11) |
| O2 | 0.0781 (16) | 0.0553 (13) | 0.0701 (15) | 0.0154 (11) | 0.0328 (13) | −0.0027 (12) |
| O3 | 0.0589 (14) | 0.0645 (13) | 0.0470 (10) | 0.0096 (11) | 0.0079 (9) | 0.0076 (10) |
| O4 | 0.0689 (15) | 0.0505 (12) | 0.0467 (12) | 0.0119 (10) | 0.0136 (11) | 0.0053 (10) |
| O5 | 0.0434 (12) | 0.0385 (10) | 0.0631 (13) | 0.0043 (8) | 0.0221 (10) | 0.0011 (9) |
| O6 | 0.0438 (12) | 0.0479 (11) | 0.0779 (15) | 0.0059 (9) | 0.0289 (11) | 0.0033 (10) |
| O7 | 0.0796 (17) | 0.0774 (15) | 0.0695 (16) | −0.0069 (13) | 0.0209 (13) | −0.0040 (13) |
| O8 | 0.0659 (16) | 0.0728 (15) | 0.0851 (18) | 0.0276 (12) | 0.0138 (13) | −0.0040 (13) |
| N1 | 0.0307 (12) | 0.0490 (13) | 0.0354 (12) | −0.0030 (10) | 0.0078 (10) | −0.0028 (10) |
| N2 | 0.0321 (12) | 0.0442 (12) | 0.0399 (12) | −0.0049 (9) | 0.0055 (10) | −0.0018 (10) |
| N3 | 0.0411 (14) | 0.0507 (13) | 0.0474 (14) | 0.0069 (11) | 0.0187 (11) | 0.0059 (11) |
| N4 | 0.0452 (14) | 0.0506 (13) | 0.0537 (14) | 0.0103 (11) | 0.0254 (12) | 0.0086 (12) |
| C1 | 0.0436 (17) | 0.0450 (15) | 0.063 (2) | −0.0082 (13) | 0.0152 (15) | −0.0032 (14) |
| C2 | 0.0427 (19) | 0.069 (2) | 0.069 (2) | −0.0175 (16) | 0.0144 (16) | −0.0054 (18) |
| C3 | 0.0347 (17) | 0.082 (2) | 0.0534 (19) | −0.0001 (16) | 0.0144 (14) | 0.0067 (17) |
| C4 | 0.0493 (19) | 0.0628 (19) | 0.061 (2) | 0.0084 (15) | 0.0184 (16) | −0.0030 (16) |
| C5 | 0.0412 (17) | 0.0498 (16) | 0.0554 (18) | −0.0030 (13) | 0.0118 (14) | −0.0066 (14) |
| C6 | 0.0377 (15) | 0.0437 (14) | 0.0388 (15) | −0.0051 (12) | 0.0131 (12) | 0.0006 (12) |
| C7 | 0.0401 (16) | 0.0377 (14) | 0.0431 (15) | −0.0042 (11) | 0.0126 (13) | 0.0014 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0372 (15) | 0.0396 (14) | 0.0453 (16) | −0.0041 (11) | 0.0106 (13) | −0.0029 (12) |
| C9 | 0.0390 (16) | 0.0398 (14) | 0.0528 (17) | −0.0060 (12) | 0.0101 (13) | −0.0069 (13) |
| C10 | 0.069 (2) | 0.0658 (19) | 0.0327 (15) | −0.0226 (16) | 0.0082 (15) | 0.0039 (14) |
| C11 | 0.0566 (19) | 0.0522 (17) | 0.0440 (16) | −0.0187 (14) | 0.0101 (14) | 0.0048 (14) |
| C12 | 0.0349 (15) | 0.0516 (16) | 0.0396 (15) | −0.0042 (12) | 0.0091 (12) | 0.0055 (12) |
| C13 | 0.105 (3) | 0.082 (3) | 0.117 (3) | 0.042 (2) | 0.087 (3) | 0.050 (2) |
| C14 | 0.092 (3) | 0.067 (2) | 0.109 (3) | 0.033 (2) | 0.072 (3) | 0.041 (2) |
| C15 | 0.0405 (16) | 0.0544 (17) | 0.0425 (16) | 0.0034 (13) | 0.0164 (13) | 0.0082 (13) |
| C16 | 0.056 (2) | 0.0467 (16) | 0.062 (2) | 0.0089 (14) | 0.0275 (16) | 0.0016 (14) |
| C17 | 0.0543 (19) | 0.0532 (17) | 0.0546 (18) | 0.0115 (14) | 0.0244 (15) | −0.0007 (14) |
| C18 | 0.058 (2) | 0.0533 (17) | 0.0430 (16) | 0.0172 (15) | 0.0255 (15) | 0.0116 (14) |
| C19 | 0.0548 (19) | 0.068 (2) | 0.0425 (17) | 0.0206 (16) | 0.0257 (15) | 0.0180 (15) |
| C20 | 0.051 (2) | 0.095 (3) | 0.0479 (19) | 0.0126 (19) | 0.0204 (16) | 0.0090 (18) |
| C21 | 0.060 (2) | 0.129 (3) | 0.050 (2) | −0.001 (2) | 0.0185 (18) | 0.009 (2) |
| C22 | 0.053 (2) | 0.179 (5) | 0.055 (2) | 0.022 (3) | 0.023 (2) | 0.046 (3) |
| C23 | 0.073 (3) | 0.147 (4) | 0.077 (3) | 0.060 (3) | 0.046 (3) | 0.057 (3) |
| C24 | 0.069 (3) | 0.087 (2) | 0.067 (2) | 0.0357 (19) | 0.040 (2) | 0.0285 (19) |
| C25 | 0.066 (2) | 0.0524 (19) | 0.0524 (19) | 0.0215 (16) | 0.0184 (18) | 0.0097 (15) |
| C26 | 0.116 (3) | 0.083 (3) | 0.058 (2) | 0.007 (2) | 0.001 (2) | 0.029 (2) |
| C27 | 0.0458 (17) | 0.0341 (13) | 0.0492 (16) | −0.0003 (12) | 0.0233 (14) | −0.0051 (12) |
| C28 | 0.097 (3) | 0.0394 (18) | 0.172 (4) | 0.0031 (18) | 0.090 (3) | 0.010 (2) |

*Geometric parameters (Å, º)*

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| Cd1—O5$^{i}$ | 2.2331 (18) | C7—C8 | 1.509 (3) |
| Cd1—N1 | 2.238 (2) | C8—C9 | 1.518 (3) |
| Cd1—N3 | 2.349 (2) | C8—H8A′ | 0.9700 |
| Cd1—O3 | 2.354 (2) | C8—H8B′ | 0.9700 |
| Cd1—O4 | 2.446 (2) | C9—H9A | 0.9700 |
| Cd1—O5 | 2.5855 (18) | C9—H9B | 0.9700 |
| Cd1—C25 | 2.749 (3) | C10—C11 | 1.342 (4) |
| O1—C7 | 1.214 (3) | C10—H10 | 0.9300 |
| O2—C18 | 1.215 (3) | C11—H11 | 0.9300 |
| O3—C25 | 1.268 (4) | C12—H12 | 0.9300 |
| O4—C25 | 1.257 (4) | C13—C14 | 1.334 (4) |
| O5—C27 | 1.275 (3) | C13—H13 | 0.9300 |
| O5—Cd1$^{i}$ | 2.2331 (18) | C14—H14 | 0.9300 |
| O6—C27 | 1.229 (3) | C15—H15 | 0.9300 |
| O7—H7A | 0.8500 | C16—C17 | 1.517 (4) |
| O7—H7B | 0.8499 | C16—H16A | 0.9700 |
| O8—H8A | 0.8500 | C16—H16B | 0.9700 |
| O8—H8B | 0.8500 | C17—C18 | 1.512 (4) |
| N1—C12 | 1.311 (3) | C17—H17A | 0.9700 |
| N1—C11 | 1.364 (3) | C17—H17B | 0.9700 |
| N2—C12 | 1.344 (3) | C18—C19 | 1.490 (4) |
| N2—C10 | 1.358 (3) | C19—C20 | 1.382 (5) |
| N2—C9 | 1.464 (3) | C19—C24 | 1.398 (4) |
| N3—C15 | 1.316 (3) | C20—C21 | 1.393 (4) |

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| N3—C14 | 1.369 (4) | C20—H20 | 0.9300 |
| N4—C15 | 1.338 (3) | C21—C22 | 1.382 (6) |
| N4—C13 | 1.359 (4) | C21—H21 | 0.9300 |
| N4—C16 | 1.455 (3) | C22—C23 | 1.371 (6) |
| C1—C2 | 1.376 (4) | C22—H22 | 0.9300 |
| C1—C6 | 1.388 (4) | C23—C24 | 1.379 (5) |
| C1—H1 | 0.9300 | C23—H23 | 0.9300 |
| C2—C3 | 1.371 (4) | C24—H24 | 0.9300 |
| C2—H2 | 0.9300 | C25—C26 | 1.514 (4) |
| C3—C4 | 1.374 (4) | C26—H26A | 0.9600 |
| C3—H3 | 0.9300 | C26—H26B | 0.9600 |
| C4—C5 | 1.386 (4) | C26—H26C | 0.9600 |
| C4—H4 | 0.9300 | C27—C28 | 1.499 (4) |
| C5—C6 | 1.386 (4) | C28—H28A | 0.9600 |
| C5—H5 | 0.9300 | C28—H28B | 0.9600 |
| C6—C7 | 1.492 (4) | C28—H28C | 0.9600 |

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| O5$^{i}$—Cd1—N1 | 100.91 (7) | C11—C10—N2 | 107.0 (2) |
| O5$^{i}$—Cd1—N3 | 115.03 (7) | C11—C10—H10 | 126.5 |
| N1—Cd1—N3 | 102.24 (8) | N2—C10—H10 | 126.5 |
| O5$^{i}$—Cd1—O3 | 105.01 (8) | C10—C11—N1 | 109.5 (2) |
| N1—Cd1—O3 | 145.14 (8) | C10—C11—H11 | 125.2 |
| N3—Cd1—O3 | 87.54 (8) | N1—C11—H11 | 125.2 |
| O5$^{i}$—Cd1—O4 | 154.40 (7) | N1—C12—N2 | 111.5 (2) |
| N1—Cd1—O4 | 93.31 (8) | N1—C12—H12 | 124.3 |
| N3—Cd1—O4 | 82.00 (7) | N2—C12—H12 | 124.3 |
| O3—Cd1—O4 | 54.55 (8) | C14—C13—N4 | 107.2 (3) |
| O5$^{i}$—Cd1—O5 | 72.10 (7) | C14—C13—H13 | 126.4 |
| N1—Cd1—O5 | 81.39 (7) | N4—C13—H13 | 126.4 |
| N3—Cd1—O5 | 170.77 (7) | C13—C14—N3 | 110.2 (3) |
| O3—Cd1—O5 | 84.80 (7) | C13—C14—H14 | 124.9 |
| O4—Cd1—O5 | 89.35 (6) | N3—C14—H14 | 124.9 |
| O5$^{i}$—Cd1—C25 | 131.37 (9) | N3—C15—N4 | 112.6 (2) |
| N1—Cd1—C25 | 119.91 (10) | N3—C15—H15 | 123.7 |
| N3—Cd1—C25 | 82.74 (8) | N4—C15—H15 | 123.7 |
| O3—Cd1—C25 | 27.40 (9) | N4—C16—C17 | 111.1 (2) |
| O4—Cd1—C25 | 27.21 (8) | N4—C16—H16A | 109.4 |
| O5—Cd1—C25 | 88.09 (8) | C17—C16—H16A | 109.4 |
| C25—O3—Cd1 | 93.93 (19) | N4—C16—H16B | 109.4 |
| C25—O4—Cd1 | 89.92 (19) | C17—C16—H16B | 109.4 |
| C27—O5—Cd1$^{i}$ | 110.77 (16) | H16A—C16—H16B | 108.0 |
| C27—O5—Cd1 | 133.36 (17) | C18—C17—C16 | 113.1 (3) |
| Cd1$^{i}$—O5—Cd1 | 107.90 (7) | C18—C17—H17A | 109.0 |
| H7A—O7—H7B | 116.4 | C16—C17—H17A | 109.0 |
| H8A—O8—H8B | 116.3 | C18—C17—H17B | 109.0 |
| C12—N1—C11 | 105.6 (2) | C16—C17—H17B | 109.0 |
| C12—N1—Cd1 | 129.21 (18) | H17A—C17—H17B | 107.8 |
| C11—N1—Cd1 | 125.20 (18) | O2—C18—C19 | 121.2 (3) |

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| C12—N2—C10 | 106.5 (2) | O2—C18—C17 | 120.7 (3) |
| C12—N2—C9 | 126.8 (2) | C19—C18—C17 | 118.0 (3) |
| C10—N2—C9 | 126.7 (2) | C20—C19—C24 | 118.8 (3) |
| C15—N3—C14 | 104.1 (2) | C20—C19—C18 | 122.9 (3) |
| C15—N3—Cd1 | 129.63 (18) | C24—C19—C18 | 118.3 (3) |
| C14—N3—Cd1 | 126.21 (19) | C19—C20—C21 | 120.7 (3) |
| C15—N4—C13 | 105.9 (2) | C19—C20—H20 | 119.7 |
| C15—N4—C16 | 127.6 (2) | C21—C20—H20 | 119.7 |
| C13—N4—C16 | 126.3 (2) | C22—C21—C20 | 119.5 (4) |
| C2—C1—C6 | 120.5 (3) | C22—C21—H21 | 120.3 |
| C2—C1—H1 | 119.7 | C20—C21—H21 | 120.3 |
| C6—C1—H1 | 119.7 | C23—C22—C21 | 120.2 (4) |
| C3—C2—C1 | 120.4 (3) | C23—C22—H22 | 119.9 |
| C3—C2—H2 | 119.8 | C21—C22—H22 | 119.9 |
| C1—C2—H2 | 119.8 | C22—C23—C24 | 120.5 (4) |
| C2—C3—C4 | 119.9 (3) | C22—C23—H23 | 119.7 |
| C2—C3—H3 | 120.1 | C24—C23—H23 | 119.7 |
| C4—C3—H3 | 120.1 | C23—C24—C19 | 120.3 (4) |
| C3—C4—C5 | 120.2 (3) | C23—C24—H24 | 119.9 |
| C3—C4—H4 | 119.9 | C19—C24—H24 | 119.9 |
| C5—C4—H4 | 119.9 | O4—C25—O3 | 121.3 (3) |
| C4—C5—C6 | 120.3 (3) | O4—C25—C26 | 119.0 (3) |
| C4—C5—H5 | 119.9 | O3—C25—C26 | 119.7 (3) |
| C6—C5—H5 | 119.9 | O4—C25—Cd1 | 62.87 (16) |
| C5—C6—C1 | 118.7 (3) | O3—C25—Cd1 | 58.67 (15) |
| C5—C6—C7 | 122.7 (2) | C26—C25—Cd1 | 173.5 (2) |
| C1—C6—C7 | 118.5 (2) | C25—C26—H26A | 109.5 |
| O1—C7—C6 | 120.6 (2) | C25—C26—H26B | 109.5 |
| O1—C7—C8 | 120.0 (2) | H26A—C26—H26B | 109.5 |
| C6—C7—C8 | 119.4 (2) | C25—C26—H26C | 109.5 |
| C7—C8—C9 | 111.6 (2) | H26A—C26—H26C | 109.5 |
| C7—C8—H8A′ | 109.3 | H26B—C26—H26C | 109.5 |
| C9—C8—H8A′ | 109.3 | O6—C27—O5 | 122.6 (2) |
| C7—C8—H8B′ | 109.3 | O6—C27—C28 | 119.4 (3) |
| C9—C8—H8B′ | 109.3 | O5—C27—C28 | 118.0 (3) |
| H8A′—C8—H8B′ | 108.0 | C27—C28—H28A | 109.5 |
| N2—C9—C8 | 111.5 (2) | C27—C28—H28B | 109.5 |
| N2—C9—H9A | 109.3 | H28A—C28—H28B | 109.5 |
| C8—C9—H9A | 109.3 | C27—C28—H28C | 109.5 |
| N2—C9—H9B | 109.3 | H28A—C28—H28C | 109.5 |
| C8—C9—H9B | 109.3 | H28B—C28—H28C | 109.5 |
| H9A—C9—H9B | 108.0 | | |

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| O5$^{i}$—Cd1—O3—C25 | −165.80 (17) | C10—N2—C9—C8 | −73.3 (4) |
| N1—Cd1—O3—C25 | −29.1 (2) | C7—C8—C9—N2 | 175.6 (2) |
| N3—Cd1—O3—C25 | 78.93 (18) | C12—N2—C10—C11 | 0.1 (3) |
| O4—Cd1—O3—C25 | −3.00 (17) | C9—N2—C10—C11 | 178.0 (3) |
| O5—Cd1—O3—C25 | −95.91 (18) | N2—C10—C11—N1 | −0.7 (4) |

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| O5$^{i}$—Cd1—O4—C25 | 44.4 (3) | C12—N1—C11—C10 | 1.1 (3) |
| N1—Cd1—O4—C25 | 168.43 (18) | Cd1—N1—C11—C10 | 179.5 (2) |
| N3—Cd1—O4—C25 | −89.67 (18) | C11—N1—C12—N2 | −1.1 (3) |
| O3—Cd1—O4—C25 | 3.02 (17) | Cd1—N1—C12—N2 | −179.42 (16) |
| O5—Cd1—O4—C25 | 87.10 (18) | C10—N2—C12—N1 | 0.6 (3) |
| O5$^{i}$—Cd1—O5—C27 | 144.8 (3) | C9—N2—C12—N1 | −177.3 (2) |
| N1—Cd1—O5—C27 | −110.7 (2) | C15—N4—C13—C14 | −0.3 (4) |
| N3—Cd1—O5—C27 | 3.1 (6) | C16—N4—C13—C14 | 174.2 (3) |
| O3—Cd1—O5—C27 | 37.2 (2) | N4—C13—C14—N3 | 0.7 (5) |
| O4—Cd1—O5—C27 | −17.2 (2) | C15—N3—C14—C13 | −0.9 (4) |
| C25—Cd1—O5—C27 | 10.0 (2) | Cd1—N3—C14—C13 | 177.8 (3) |
| O5$^{i}$—Cd1—O5—Cd1$^{i}$ | 0.0 | C14—N3—C15—N4 | 0.7 (4) |
| N1—Cd1—O5—Cd1$^{i}$ | 104.48 (9) | Cd1—N3—C15—N4 | −177.87 (18) |
| N3—Cd1—O5—Cd1$^{i}$ | −141.7 (4) | C13—N4—C15—N3 | −0.3 (4) |
| O3—Cd1—O5—Cd1$^{i}$ | −107.62 (9) | C16—N4—C15—N3 | −174.7 (3) |
| O4—Cd1—O5—Cd1$^{i}$ | −162.07 (8) | C15—N4—C16—C17 | 100.1 (3) |
| C25—Cd1—O5—Cd1$^{i}$ | −134.88 (10) | C13—N4—C16—C17 | −73.3 (4) |
| O5$^{i}$—Cd1—N1—C12 | 164.3 (2) | N4—C16—C17—C18 | 171.1 (2) |
| N3—Cd1—N1—C12 | −76.8 (2) | C16—C17—C18—O2 | 0.8 (4) |
| O3—Cd1—N1—C12 | 26.7 (3) | C16—C17—C18—C19 | −178.9 (2) |
| O4—Cd1—N1—C12 | 5.7 (2) | O2—C18—C19—C20 | −178.7 (3) |
| O5—Cd1—N1—C12 | 94.5 (2) | C17—C18—C19—C20 | 1.0 (4) |
| C25—Cd1—N1—C12 | 11.8 (3) | O2—C18—C19—C24 | 1.5 (4) |
| O5$^{i}$—Cd1—N1—C11 | −13.7 (2) | C17—C18—C19—C24 | −178.7 (3) |
| N3—Cd1—N1—C11 | 105.1 (2) | C24—C19—C20—C21 | 0.1 (5) |
| O3—Cd1—N1—C11 | −151.3 (2) | C18—C19—C20—C21 | −179.6 (3) |
| O4—Cd1—N1—C11 | −172.4 (2) | C19—C20—C21—C22 | 0.4 (5) |
| O5—Cd1—N1—C11 | −83.5 (2) | C20—C21—C22—C23 | −0.8 (6) |
| C25—Cd1—N1—C11 | −166.3 (2) | C21—C22—C23—C24 | 0.7 (6) |
| O5$^{i}$—Cd1—N3—C15 | 25.8 (3) | C22—C23—C24—C19 | −0.1 (5) |
| N1—Cd1—N3—C15 | −82.6 (2) | C20—C19—C24—C23 | −0.3 (5) |
| O3—Cd1—N3—C15 | 131.2 (2) | C18—C19—C24—C23 | 179.5 (3) |
| O4—Cd1—N3—C15 | −174.2 (3) | Cd1—O4—C25—O3 | −5.3 (3) |
| O5—Cd1—N3—C15 | 165.2 (3) | Cd1—O4—C25—C26 | 172.9 (3) |
| C25—Cd1—N3—C15 | 158.3 (3) | Cd1—O3—C25—O4 | 5.6 (3) |
| O5$^{i}$—Cd1—N3—C14 | −152.5 (3) | Cd1—O3—C25—C26 | −172.7 (3) |
| N1—Cd1—N3—C14 | 99.1 (3) | O5$^{i}$—Cd1—C25—O4 | −156.24 (15) |
| O3—Cd1—N3—C14 | −47.1 (3) | N1—Cd1—C25—O4 | −13.4 (2) |
| O4—Cd1—N3—C14 | 7.5 (3) | N3—Cd1—C25—O4 | 86.62 (18) |
| O5—Cd1—N3—C14 | −13.1 (6) | O3—Cd1—C25—O4 | −174.6 (3) |
| C25—Cd1—N3—C14 | −20.0 (3) | O5—Cd1—C25—O4 | −92.28 (17) |
| C6—C1—C2—C3 | 0.0 (5) | O5$^{i}$—Cd1—C25—O3 | 18.4 (2) |
| C1—C2—C3—C4 | 0.2 (5) | N1—Cd1—C25—O3 | 161.30 (16) |
| C2—C3—C4—C5 | −0.5 (5) | N3—Cd1—C25—O3 | −98.73 (18) |
| C3—C4—C5—C6 | 0.8 (5) | O4—Cd1—C25—O3 | 174.6 (3) |
| C4—C5—C6—C1 | −0.6 (4) | O5—Cd1—C25—O3 | 82.37 (17) |
| C4—C5—C6—C7 | −179.9 (3) | O5$^{i}$—Cd1—C25—C26 | 95 (2) |
| C2—C1—C6—C5 | 0.2 (4) | N1—Cd1—C25—C26 | −122 (2) |

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| C2—C1—C6—C7 | 179.6 (3) | N3—Cd1—C25—C26 | −22 (2) |
| C5—C6—C7—O1 | −179.0 (3) | O3—Cd1—C25—C26 | 77 (2) |
| C1—C6—C7—O1 | 1.7 (4) | O4—Cd1—C25—C26 | −108 (2) |
| C5—C6—C7—C8 | 0.2 (4) | O5—Cd1—C25—C26 | 159 (2) |
| C1—C6—C7—C8 | −179.1 (3) | Cd1$^{i}$—O5—C27—O6 | 8.6 (3) |
| O1—C7—C8—C9 | −3.1 (4) | Cd1—O5—C27—O6 | −135.5 (2) |
| C6—C7—C8—C9 | 177.7 (2) | Cd1$^{i}$—O5—C27—C28 | −170.7 (2) |
| C12—N2—C9—C8 | 104.2 (3) | Cd1—O5—C27—C28 | 45.2 (4) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O7—H7*A*···O3$^{ii}$ | 0.85 | 2.11 | 2.949 (3) | 169 |
| O7—H7*B*···O4$^{iii}$ | 0.85 | 1.99 | 2.829 (3) | 171 |
| O8—H8*B*···O6$^{iii}$ | 0.85 | 2.03 | 2.838 (3) | 159 |
| O8—H8*A*···O7$^{iv}$ | 0.85 | 1.97 | 2.818 (3) | 174 |

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