

## Diaqua(nitrato- $\kappa^2O,O'$ )[2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline- $\kappa^2N,N'$ ]cadmium(II) nitrate

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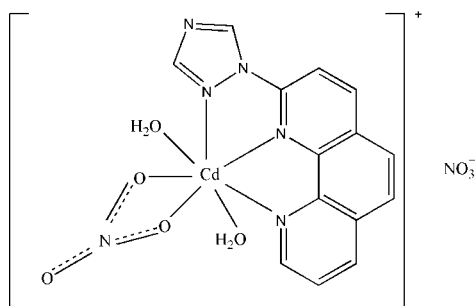
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.104; data-to-parameter ratio = 12.2.

In the title complex,  $[\text{Cd}(\text{C}_{14}\text{H}_9\text{N}_5)(\text{NO}_3)(\text{H}_2\text{O})_2]\text{NO}_3$ , the  $\text{Cd}^{\text{II}}$  ion is coordinated in a distorted pentagonal-bipyramidal geometry. The equatorial sites are occupied by a 2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline ligand in a tridentate coordination mode and a bis-chelating nitrate ligand. Two aqua ligands are coordinated at the axial sites. All non-H atoms in the equatorial plane are co-planar within 0.0673 Å. In the crystal, intermolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds connect the components into a two-dimensional network parallel to (001). In addition, there is a  $\pi-\pi$  stacking interaction between symmetry-related benzene rings, with a centroid-centroid distance of 3.598 (3) Å.

### Related literature

For related structures, see: Li (2009); Xie *et al.* (2009).



### Experimental

#### Crystal data

$[\text{Cd}(\text{C}_{14}\text{H}_9\text{N}_5)(\text{NO}_3)(\text{H}_2\text{O})_2]\text{NO}_3$	$\gamma = 83.375$ (3) $^\circ$
$M_r = 519.71$	$V = 900.4$ (3) Å <sup>3</sup>
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.9934$ (18) Å	Mo $K\alpha$ radiation
$b = 9.1995$ (19) Å	$\mu = 1.28$ mm <sup>-1</sup>
$c = 11.460$ (2) Å	$T = 298$ K
$\alpha = 88.334$ (3) $^\circ$	$0.25 \times 0.10 \times 0.08$ mm
$\beta = 72.946$ (3) $^\circ$	

#### Data collection

Bruker SMART APEX CCD diffractometer	4496 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3311 independent reflections
$T_{\text{min}} = 0.741$ , $T_{\text{max}} = 0.905$	2954 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.020$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	271 parameters
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.78$ e Å <sup>-3</sup>
3311 reflections	$\Delta\rho_{\text{min}} = -0.56$ e Å <sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O8—H5 $\cdots$ O5 <sup>i</sup>	0.75	2.05	2.752 (6)	156
O8—H4 $\cdots$ O2 <sup>ii</sup>	0.86	2.03	2.865 (5)	163
O7—H7 $\cdots$ O3 <sup>iii</sup>	0.78	2.59	3.269 (6)	147
O7—H7 $\cdots$ O1 <sup>iii</sup>	0.78	2.22	2.966 (5)	160
O7—H6 $\cdots$ N5 <sup>iv</sup>	0.99	2.47	3.420 (6)	162
O7—H6 $\cdots$ O6 <sup>iv</sup>	0.99	2.45	3.227 (6)	135
O7—H6 $\cdots$ O4 <sup>iv</sup>	0.99	1.83	2.802 (6)	167

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH5140).

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**supplementary materials**

*Acta Cryst.* (2010). E66, m1392 [ doi:10.1107/S1600536810039735 ]

**Diaqua(nitrato- $\kappa^2O,O'$ )[2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline- $\kappa^2N,N'$ ]cadmium(II) nitrate**

**S. G. Zhang and H. M. Zhang**

**Comment**

Derivatives of 1,10-phenanthroline play an important role in modern coordination chemistry and to our knowledge only two complexes with 2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline as ligand have been published up to date (Li, 2009; Xie *et al.* 2009). Our interest in the correlation between the coordination geometry and the counter ion resulted in us synthesizing the title complex and herein we report its crystal structure.

The molecular structure of the title compound is shown in Fig. 1. The Cd<sup>II</sup> ion is in a distorted pentagonal bipyramidal coordination environment, with two H<sub>2</sub>O ligands in the axial positions. Except for the two water molecules, all non-hydrogen atoms of the cation define a plane within 0.0673 Å with a maximum deviation of -0.1532 (39) Å for atom N5. In the crystal structure, hydrogen bonds involving coordinated water molecules, nitrato ligands and nitrate anions connect the components of the structure into a two-dimensional network parallel to (001). In addition, there is a  $\pi$ - $\pi$  stacking interaction involving symmetry-related complexes, the relevant distances being  $Cg1 \cdots Cg1^i = 3.598(3)$  Å and  $Cg1 \cdots Cg1^i_{\text{perp}} = 3.428$  Å [symmetry code: (i) 1 - *x*, -*y*, 1 - *z*; Cg1 is the centroid of C4—C9 ring].

**Experimental**

A 5 ml water solution of Cd(NO<sub>3</sub>)<sub>2</sub>·4H<sub>2</sub>O (0.0742 g, 0.240 mmol) was added into a 15 ml methanol solution containing 2-(1*H*-1,2,4-triazol-1-yl)-1,10-phenanthroline (0.0598 g, 0.242 mmol) and the mixture was stirred for a few minutes. Colourless single crystals were obtained after the filtrate had been allowed to stand at room temperature for two weeks.

**Refinement**

The water H atoms were located in a difference Fourier map and refined as riding in their 'as found' positions with  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{O})$ . Other H atoms were placed in calculated positions and refined as riding with C—H = 0.93 Å,  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ .

**Figures**

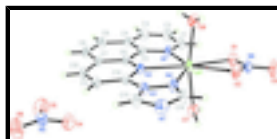


Fig. 1. The asymmetric unit of the title compound with displacement ellipsoids shown at the 30% probability level

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### Crystal data

$[\text{Cd}(\text{C}_{14}\text{H}_9\text{N}_5)(\text{NO}_3)(\text{H}_2\text{O})_2]\text{NO}_3$	$Z = 2$
$M_r = 519.71$	$F(000) = 516$
Triclinic, $P\bar{1}$	$D_x = 1.917 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 8.9934 (18) \text{ \AA}$	Cell parameters from 1655 reflections
$b = 9.1995 (19) \text{ \AA}$	$\theta = 2.6\text{--}24.8^\circ$
$c = 11.460 (2) \text{ \AA}$	$\mu = 1.28 \text{ mm}^{-1}$
$\alpha = 88.334 (3)^\circ$	$T = 298 \text{ K}$
$\beta = 72.946 (3)^\circ$	Block, colorless
$\gamma = 83.375 (3)^\circ$	$0.25 \times 0.10 \times 0.08 \text{ mm}$
$V = 900.4 (3) \text{ \AA}^3$	

### Data collection

Bruker SMART APEX CCD diffractometer	3311 independent reflections
Radiation source: fine-focus sealed tube graphite	2954 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.020$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 25.8^\circ$ , $\theta_{\text{min}} = 1.9^\circ$
$T_{\text{min}} = 0.741$ , $T_{\text{max}} = 0.905$	$h = -10 \rightarrow 10$
4496 measured reflections	$k = -9 \rightarrow 11$
	$l = -14 \rightarrow 12$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.104$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.1075P]$
3311 reflections	where $P = (F_o^2 + 2F_c^2)/3$
271 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.78 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.56 \text{ e \AA}^{-3}$

### 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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4138 (6)	-0.0355 (5)	0.8867 (5)	0.0444 (12)
H1	0.3374	-0.0416	0.9611	0.053*
C2	0.5485 (7)	-0.1354 (6)	0.8625 (5)	0.0556 (14)
H2	0.5602	-0.2068	0.9192	0.067*
C3	0.6599 (6)	-0.1269 (6)	0.7571 (5)	0.0528 (14)
H3	0.7517	-0.1907	0.7414	0.063*
C4	0.6401 (5)	-0.0228 (5)	0.6697 (4)	0.0400 (11)
C5	0.5015 (5)	0.0732 (5)	0.7005 (4)	0.0337 (10)
C6	0.4752 (5)	0.1791 (5)	0.6135 (4)	0.0325 (10)
C7	0.5814 (5)	0.1851 (5)	0.4961 (4)	0.0365 (10)
C8	0.7209 (5)	0.0835 (6)	0.4682 (5)	0.0463 (13)
H8	0.7933	0.0848	0.3914	0.056*
C9	0.7484 (6)	-0.0130 (6)	0.5511 (5)	0.0506 (14)
H9	0.8411	-0.0758	0.5308	0.061*
C10	0.5412 (6)	0.2866 (6)	0.4149 (4)	0.0432 (12)
H10	0.6071	0.2899	0.3356	0.052*
C11	0.4082 (6)	0.3809 (5)	0.4486 (4)	0.0404 (11)
H11	0.3822	0.4497	0.3946	0.048*
C12	0.3123 (5)	0.3697 (5)	0.5679 (4)	0.0333 (10)
C13	0.1087 (6)	0.5780 (5)	0.5609 (5)	0.0439 (12)
H13	0.1516	0.6105	0.4818	0.053*
C14	-0.0353 (6)	0.5529 (5)	0.7377 (5)	0.0457 (12)
H15	-0.1196	0.5684	0.8078	0.055*
Cd1	0.17488 (4)	0.24849 (4)	0.84349 (3)	0.03544 (14)
N1	0.3893 (4)	0.0667 (4)	0.8096 (3)	0.0354 (9)
N2	0.3429 (4)	0.2738 (4)	0.6467 (3)	0.0326 (8)
N3	0.1732 (4)	0.4647 (4)	0.6135 (3)	0.0358 (9)
N4	0.0804 (4)	0.4489 (4)	0.7295 (3)	0.0412 (9)
N5	0.3227 (5)	0.6794 (5)	0.2041 (4)	0.0526 (11)
N6	-0.0540 (5)	0.2346 (5)	1.0734 (4)	0.0466 (11)
N7	-0.0228 (5)	0.6358 (5)	0.6366 (4)	0.0532 (11)
O1	0.0636 (4)	0.1389 (4)	1.0457 (3)	0.0549 (9)
O2	-0.0577 (4)	0.3376 (4)	1.0003 (3)	0.0519 (9)
O3	-0.1586 (5)	0.2266 (5)	1.1677 (4)	0.0750 (13)
O4	0.2077 (5)	0.7114 (5)	0.2931 (4)	0.0688 (12)
O5	0.4194 (5)	0.5758 (6)	0.2111 (4)	0.0840 (15)
O6	0.3399 (6)	0.7527 (6)	0.1125 (4)	0.0923 (16)
O7	0.0187 (4)	0.1051 (4)	0.7810 (3)	0.0493 (9)

## supplementary materials

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H6	-0.0719	0.1640	0.7649	0.074*
H7	0.0163	0.0305	0.8149	0.074*
O8	0.2817 (4)	0.4079 (4)	0.9389 (3)	0.0524 (9)
H4	0.2302	0.4922	0.9605	0.079*
H5	0.3553	0.4366	0.9016	0.079*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.048 (3)	0.039 (3)	0.041 (3)	0.007 (2)	-0.009 (2)	0.005 (2)
C2	0.067 (4)	0.044 (3)	0.051 (3)	0.016 (3)	-0.019 (3)	0.009 (2)
C3	0.049 (3)	0.046 (3)	0.058 (3)	0.016 (3)	-0.016 (3)	-0.002 (3)
C4	0.033 (2)	0.037 (3)	0.047 (3)	0.005 (2)	-0.010 (2)	-0.009 (2)
C5	0.034 (2)	0.029 (2)	0.035 (2)	0.0005 (19)	-0.0067 (19)	-0.0042 (18)
C6	0.028 (2)	0.032 (2)	0.034 (2)	0.0007 (19)	-0.0043 (18)	-0.0033 (18)
C7	0.033 (2)	0.037 (3)	0.034 (2)	-0.006 (2)	0.0010 (19)	-0.0066 (19)
C8	0.034 (3)	0.050 (3)	0.043 (3)	0.003 (2)	0.007 (2)	-0.016 (2)
C9	0.030 (3)	0.054 (3)	0.058 (3)	0.009 (2)	-0.001 (2)	-0.019 (3)
C10	0.044 (3)	0.049 (3)	0.026 (2)	-0.006 (2)	0.006 (2)	-0.002 (2)
C11	0.048 (3)	0.040 (3)	0.029 (2)	-0.008 (2)	-0.005 (2)	0.0066 (19)
C12	0.035 (2)	0.028 (2)	0.033 (2)	-0.0020 (19)	-0.0048 (19)	-0.0012 (18)
C13	0.051 (3)	0.034 (3)	0.046 (3)	0.003 (2)	-0.017 (2)	0.011 (2)
C14	0.044 (3)	0.037 (3)	0.048 (3)	0.011 (2)	-0.007 (2)	0.004 (2)
Cd1	0.0326 (2)	0.0334 (2)	0.0298 (2)	0.00505 (14)	0.00361 (13)	0.00419 (13)
N1	0.0320 (19)	0.037 (2)	0.032 (2)	0.0049 (17)	-0.0044 (16)	0.0055 (16)
N2	0.0308 (19)	0.031 (2)	0.030 (2)	0.0008 (16)	-0.0023 (16)	0.0008 (15)
N3	0.036 (2)	0.031 (2)	0.037 (2)	0.0000 (17)	-0.0067 (17)	0.0050 (16)
N4	0.042 (2)	0.036 (2)	0.035 (2)	0.0051 (18)	0.0005 (17)	0.0052 (16)
N5	0.052 (3)	0.055 (3)	0.053 (3)	-0.013 (2)	-0.017 (2)	0.017 (2)
N6	0.047 (2)	0.046 (3)	0.036 (2)	-0.014 (2)	0.0107 (19)	-0.0077 (19)
N7	0.051 (3)	0.044 (3)	0.060 (3)	0.011 (2)	-0.016 (2)	0.006 (2)
O1	0.059 (2)	0.046 (2)	0.047 (2)	0.0010 (19)	0.0014 (18)	0.0038 (16)
O2	0.050 (2)	0.043 (2)	0.049 (2)	0.0030 (17)	0.0043 (17)	0.0016 (17)
O3	0.068 (3)	0.078 (3)	0.052 (3)	-0.016 (2)	0.027 (2)	0.000 (2)
O4	0.058 (2)	0.088 (3)	0.055 (2)	-0.015 (2)	-0.006 (2)	0.010 (2)
O5	0.061 (3)	0.088 (4)	0.091 (3)	0.010 (3)	-0.014 (2)	0.034 (3)
O6	0.095 (4)	0.106 (4)	0.063 (3)	0.003 (3)	-0.012 (3)	0.041 (3)
O7	0.0464 (19)	0.041 (2)	0.057 (2)	-0.0010 (16)	-0.0103 (17)	0.0037 (16)
O8	0.048 (2)	0.045 (2)	0.059 (2)	0.0000 (17)	-0.0091 (18)	-0.0049 (17)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—N1	1.316 (6)	C13—N7	1.309 (7)
C1—C2	1.396 (7)	C13—N3	1.347 (6)
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.331 (7)	C14—N4	1.313 (6)
C2—H2	0.9300	C14—N7	1.352 (7)
C3—C4	1.401 (7)	C14—H15	0.9300
C3—H3	0.9300	Cd1—O7	2.301 (4)

C4—C5	1.401 (6)	Cd1—O8	2.303 (4)
C4—C9	1.429 (7)	Cd1—N2	2.340 (3)
C5—N1	1.362 (5)	Cd1—N1	2.350 (4)
C5—C6	1.424 (6)	Cd1—O2	2.400 (3)
C6—N2	1.353 (5)	Cd1—N4	2.445 (4)
C6—C7	1.407 (6)	Cd1—O1	2.475 (4)
C7—C10	1.392 (7)	N3—N4	1.361 (5)
C7—C8	1.436 (6)	N5—O6	1.212 (6)
C8—C9	1.337 (8)	N5—O5	1.231 (6)
C8—H8	0.9300	N5—O4	1.235 (6)
C9—H9	0.9300	N6—O3	1.214 (5)
C10—C11	1.357 (7)	N6—O2	1.251 (6)
C10—H10	0.9300	N6—O1	1.265 (5)
C11—C12	1.395 (6)	O7—H6	0.9858
C11—H11	0.9300	O7—H7	0.7785
C12—N2	1.309 (6)	O8—H4	0.8595
C12—N3	1.411 (6)	O8—H5	0.7473
N1—C1—C2	123.4 (5)	O7—Cd1—N1	94.70 (13)
N1—C1—H1	118.3	O8—Cd1—N1	94.71 (13)
C2—C1—H1	118.3	N2—Cd1—N1	70.66 (12)
C3—C2—C1	119.1 (5)	O7—Cd1—O2	86.19 (13)
C3—C2—H2	120.4	O8—Cd1—O2	81.33 (13)
C1—C2—H2	120.4	N2—Cd1—O2	148.68 (12)
C2—C3—C4	120.5 (5)	N1—Cd1—O2	140.60 (13)
C2—C3—H3	119.7	O7—Cd1—N4	87.39 (14)
C4—C3—H3	119.7	O8—Cd1—N4	91.19 (14)
C5—C4—C3	117.0 (5)	N2—Cd1—N4	66.93 (12)
C5—C4—C9	118.8 (4)	N1—Cd1—N4	137.57 (12)
C3—C4—C9	124.2 (4)	O2—Cd1—N4	81.82 (12)
N1—C5—C4	122.4 (4)	O7—Cd1—O1	84.17 (13)
N1—C5—C6	118.8 (4)	O8—Cd1—O1	87.88 (13)
C4—C5—C6	118.9 (4)	N2—Cd1—O1	158.95 (13)
N2—C6—C7	120.6 (4)	N1—Cd1—O1	88.53 (12)
N2—C6—C5	117.8 (4)	O2—Cd1—O1	52.30 (12)
C7—C6—C5	121.6 (4)	N4—Cd1—O1	133.72 (12)
C10—C7—C6	117.4 (4)	C1—N1—C5	117.6 (4)
C10—C7—C8	125.0 (4)	C1—N1—Cd1	126.6 (3)
C6—C7—C8	117.5 (4)	C5—N1—Cd1	115.7 (3)
C9—C8—C7	121.1 (4)	C12—N2—C6	119.6 (4)
C9—C8—H8	119.5	C12—N2—Cd1	123.5 (3)
C7—C8—H8	119.5	C6—N2—Cd1	116.9 (3)
C8—C9—C4	122.1 (4)	C13—N3—N4	108.9 (4)
C8—C9—H9	118.9	C13—N3—C12	130.9 (4)
C4—C9—H9	118.9	N4—N3—C12	120.2 (4)
C11—C10—C7	121.6 (4)	C14—N4—N3	102.6 (4)
C11—C10—H10	119.2	C14—N4—Cd1	142.7 (3)
C7—C10—H10	119.2	N3—N4—Cd1	114.7 (3)
C10—C11—C12	116.8 (4)	O6—N5—O5	121.3 (5)
C10—C11—H11	121.6	O6—N5—O4	119.3 (5)

## supplementary materials

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C12—C11—H11	121.6	O5—N5—O4	119.4 (5)
N2—C12—C11	123.8 (4)	O3—N6—O2	121.5 (5)
N2—C12—N3	114.6 (4)	O3—N6—O1	121.1 (5)
C11—C12—N3	121.6 (4)	O2—N6—O1	117.4 (4)
N7—C13—N3	110.5 (4)	C13—N7—C14	103.0 (4)
N7—C13—H13	124.8	N6—O1—Cd1	93.0 (3)
N3—C13—H13	124.8	N6—O2—Cd1	97.0 (3)
N4—C14—N7	115.0 (5)	Cd1—O7—H6	111.8
N4—C14—H15	122.5	Cd1—O7—H7	110.1
N7—C14—H15	122.5	H6—O7—H7	125.4
O7—Cd1—O8	167.51 (12)	Cd1—O8—H4	117.9
O7—Cd1—N2	94.13 (12)	Cd1—O8—H5	116.9
O8—Cd1—N2	96.72 (13)	H4—O8—H5	95.7
N1—C1—C2—C3	0.9 (9)	O8—Cd1—N2—C12	-91.5 (4)
C1—C2—C3—C4	-2.3 (9)	N1—Cd1—N2—C12	175.9 (4)
C2—C3—C4—C5	2.1 (8)	O2—Cd1—N2—C12	-7.1 (5)
C2—C3—C4—C9	-175.3 (5)	N4—Cd1—N2—C12	-3.1 (3)
C3—C4—C5—N1	-0.4 (7)	O1—Cd1—N2—C12	166.8 (4)
C9—C4—C5—N1	177.1 (4)	O7—Cd1—N2—C6	-95.1 (3)
C3—C4—C5—C6	-178.9 (5)	O8—Cd1—N2—C6	91.0 (3)
C9—C4—C5—C6	-1.4 (7)	N1—Cd1—N2—C6	-1.6 (3)
N1—C5—C6—N2	3.6 (6)	O2—Cd1—N2—C6	175.4 (3)
C4—C5—C6—N2	-177.9 (4)	N4—Cd1—N2—C6	179.5 (3)
N1—C5—C6—C7	-175.7 (4)	O1—Cd1—N2—C6	-10.6 (6)
C4—C5—C6—C7	2.8 (7)	N7—C13—N3—N4	-0.7 (6)
N2—C6—C7—C10	-3.0 (7)	N7—C13—N3—C12	179.5 (5)
C5—C6—C7—C10	176.2 (5)	N2—C12—N3—C13	177.4 (5)
N2—C6—C7—C8	178.6 (4)	C11—C12—N3—C13	-1.7 (8)
C5—C6—C7—C8	-2.2 (7)	N2—C12—N3—N4	-2.3 (6)
C10—C7—C8—C9	-178.3 (5)	C11—C12—N3—N4	178.5 (4)
C6—C7—C8—C9	0.0 (7)	N7—C14—N4—N3	-1.0 (6)
C7—C8—C9—C4	1.5 (8)	N7—C14—N4—Cd1	-179.5 (4)
C5—C4—C9—C8	-0.8 (8)	C13—N3—N4—C14	1.0 (5)
C3—C4—C9—C8	176.5 (5)	C12—N3—N4—C14	-179.2 (4)
C6—C7—C10—C11	2.8 (7)	C13—N3—N4—Cd1	180.0 (3)
C8—C7—C10—C11	-178.9 (5)	C12—N3—N4—Cd1	-0.2 (5)
C7—C10—C11—C12	-1.0 (7)	O7—Cd1—N4—C14	84.3 (6)
C10—C11—C12—N2	-0.8 (7)	O8—Cd1—N4—C14	-83.3 (6)
C10—C11—C12—N3	178.3 (4)	N2—Cd1—N4—C14	179.9 (6)
C2—C1—N1—C5	0.7 (8)	N1—Cd1—N4—C14	178.4 (5)
C2—C1—N1—Cd1	-176.5 (4)	O2—Cd1—N4—C14	-2.2 (6)
C4—C5—N1—C1	-0.9 (7)	O1—Cd1—N4—C14	4.9 (7)
C6—C5—N1—C1	177.6 (4)	O7—Cd1—N4—N3	-94.1 (3)
C4—C5—N1—Cd1	176.6 (3)	O8—Cd1—N4—N3	98.3 (3)
C6—C5—N1—Cd1	-5.0 (5)	N2—Cd1—N4—N3	1.5 (3)
O7—Cd1—N1—C1	-86.6 (4)	N1—Cd1—N4—N3	0.0 (4)
O8—Cd1—N1—C1	85.1 (4)	O2—Cd1—N4—N3	179.4 (3)
N2—Cd1—N1—C1	-179.4 (4)	O1—Cd1—N4—N3	-173.5 (3)
O2—Cd1—N1—C1	3.1 (5)	N3—C13—N7—C14	0.1 (6)



N4—Cd1—N1—C1	-177.9 (4)	N4—C14—N7—C13	0.6 (7)
O1—Cd1—N1—C1	-2.6 (4)	O3—N6—O1—Cd1	175.4 (4)
O7—Cd1—N1—C5	96.1 (3)	O2—N6—O1—Cd1	-4.9 (4)
O8—Cd1—N1—C5	-92.1 (3)	O7—Cd1—O1—N6	-86.8 (3)
N2—Cd1—N1—C5	3.4 (3)	O8—Cd1—O1—N6	83.5 (3)
O2—Cd1—N1—C5	-174.1 (3)	N2—Cd1—O1—N6	-173.2 (3)
N4—Cd1—N1—C5	4.9 (4)	N1—Cd1—O1—N6	178.3 (3)
O1—Cd1—N1—C5	-179.8 (3)	O2—Cd1—O1—N6	2.8 (3)
C11—C12—N2—C6	0.5 (7)	N4—Cd1—O1—N6	-6.1 (4)
N3—C12—N2—C6	-178.6 (4)	O3—N6—O2—Cd1	-175.2 (4)
C11—C12—N2—Cd1	-176.8 (3)	O1—N6—O2—Cd1	5.1 (5)
N3—C12—N2—Cd1	4.0 (5)	O7—Cd1—O2—N6	82.7 (3)
C7—C6—N2—C12	1.4 (6)	O8—Cd1—O2—N6	-96.9 (3)
C5—C6—N2—C12	-177.9 (4)	N2—Cd1—O2—N6	174.4 (3)
C7—C6—N2—Cd1	179.0 (3)	N1—Cd1—O2—N6	-10.1 (4)
C5—C6—N2—Cd1	-0.3 (5)	N4—Cd1—O2—N6	170.6 (3)
O7—Cd1—N2—C12	82.3 (4)	O1—Cd1—O2—N6	-2.9 (3)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O8—H5...O5 <sup>i</sup>	0.75	2.05	2.752 (6)	156
O8—H4...O2 <sup>ii</sup>	0.86	2.03	2.865 (5)	163
O7—H7...O3 <sup>iii</sup>	0.78	2.59	3.269 (6)	147
O7—H7...O1 <sup>iii</sup>	0.78	2.22	2.966 (5)	160
O7—H6...N5 <sup>iv</sup>	0.99	2.47	3.420 (6)	162
O7—H6...O6 <sup>iv</sup>	0.99	2.45	3.227 (6)	135
O7—H6...O4 <sup>iv</sup>	0.99	1.83	2.802 (6)	167

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

Fig. 1

