metal-organic compounds

Diaquabis[5-(pyrazin-2-yl-κN^1)-3-(pyridin-3-yl)-1,2,4-triazolido-κN^1]-cadmium

Jing-Jing Yang and Jun Zhao*

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In the title compound, $[Cd(C_{11}H_7N_6)_2(H_2O)_2]$, the Cd^{II} cation is located on an inversion center and is coordinated by four N atoms from two 5-(pyrazin-2-yl)-3-(pyridin-3-yl)-1,2,4-triazolide anions and two water molecules in a distorted octahedral geometry. The triazolide ligand is nearly planar: the central triazole ring is oriented at dihedral angles of 4.63 (13) and 8.41 (13)° with respect to the pyrazine and pyridine rings. Intermolecular O—H···N hydrogen bonds link the molecules into a two-dimensional supramolecular network parallel to (001).

Related literature

For background to metal-organic frameworks, see: Kitagawa *et al.* (2004). For 1,2,4-triazole derivatives, see: Chen *et al.* (2006); Zhang *et al.* (2005).
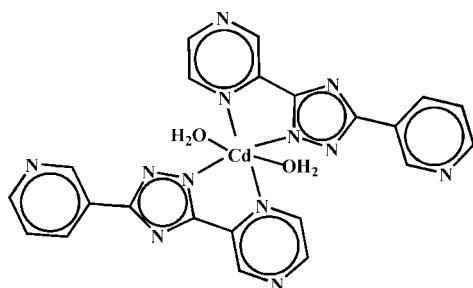
Experimental

Crystal data

$[Cd(C_{11}H_7N_6)_2(H_2O)_2]$
$M_r = 594.88$
Monoclinic, $P2_1/c$
$a = 8.640$ (5) Å
$b = 5.684$ (3) Å
$c = 23.157$ (13) Å
$\beta = 99.102$ (6)°
$V = 1122.9$ (11) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.02$ mm^{-1}
$T = 296$ K
$0.24 \times 0.21 \times 0.20$ mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.782$, $T_{max} = 0.815$
11387 measured reflections
2571 independent reflections
2251 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.081$
$S = 1.09$
2571 reflections
175 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O1	2.312 (2)	Cd1—N3	2.323 (2)
Cd1—N1	2.397 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N6^i	0.85 (2)	1.95 (2)	2.751 (3)	157 (3)
O1—H1B···N4^{ii}	0.86 (2)	1.91 (2)	2.763 (3)	173 (3)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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*.

References

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Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
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Diaquabis[5-(pyrazin-2-yl-κN^1)-3-(pyridin-3-yl)-1,2,4-triazolido-κN^1]cadmium

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S1. Comment

Much effort has been focused on the design and controlled synthesis of metal-organic frameworks or coordination polymers (Kitagawa *et al.*, 2004). 1,2,4-triazole derivatives have received considerable attention, owing to the variety of their coordination modes, and structural features (Chen *et al.*, 2006; Zhang *et al.*, 2005). During the synthesis of polymeric complexes using 2-(5-(pyridin-3-yl)-4*H*-1,2,4-triazol-3-yl)pyrazine as bridging ligand and, to our surprise, the title monomeric Cd(II) complex was obtained. The title complex, is a crstallographically centrosymmetric mononuclear complex. The Cd^{II} cation, which is located on a centre of inversion, is six-coordinated by four N atoms from two chelating 2-(5-(pyridin-3-yl)-1,2,4-triazolido-3-yl)pyrazine ligands and two water O atoms, resulting into a distored octahedral geometry (Fig. 1). In the crystal, intermolecular O–H⋯N hydrogen bonding interactions (Table 2) link the title complex into a two-dimensional supramolecular network (Fig. 2).

S2. Experimental

A mixture of 2-(5-(pyridin-3-yl)-4*H*-1,2,4-triazol-3-yl)pyrazine (0.0224 g, 0.1 mmol), Cd(CH$_3$COO)$_2$.2H$_2$O (0.0266 g, 0.1 mmol), water (10 mL) was stired vigorously for 30 min and then sealed in a Teflon-lined stainless-steel autoclave. The autoclave was heated and maintained at 413 K for 3 d, and then cooled to room temperature at 5 K h^{-1} to obtain prism crystals suitable for X-ray analysis.

S3. Refinement

Water H atoms were located in a difference Fourier map and refined with O–H restraint of 0.85±0.01 Å, $U_{iso}(H) = 1.5$ $U_{eq}(O)$. Other H-atoms were positioned geometrically and refined using a riding model with C–H = 0.93 Å, $U_{iso}(H) = 1.2$ $U_{eq}(C)$.
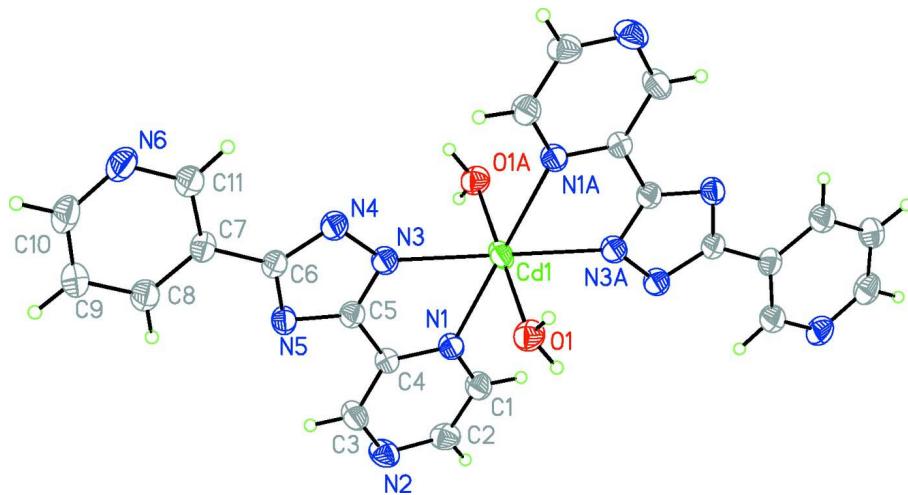
Figure 1

The *ORTEP* representation of the structure of the title compound showing the atomic numbering and 50% probability displacement ellipsoids [symmetry code: A: -*x*,-*y* + 2,-*z*].
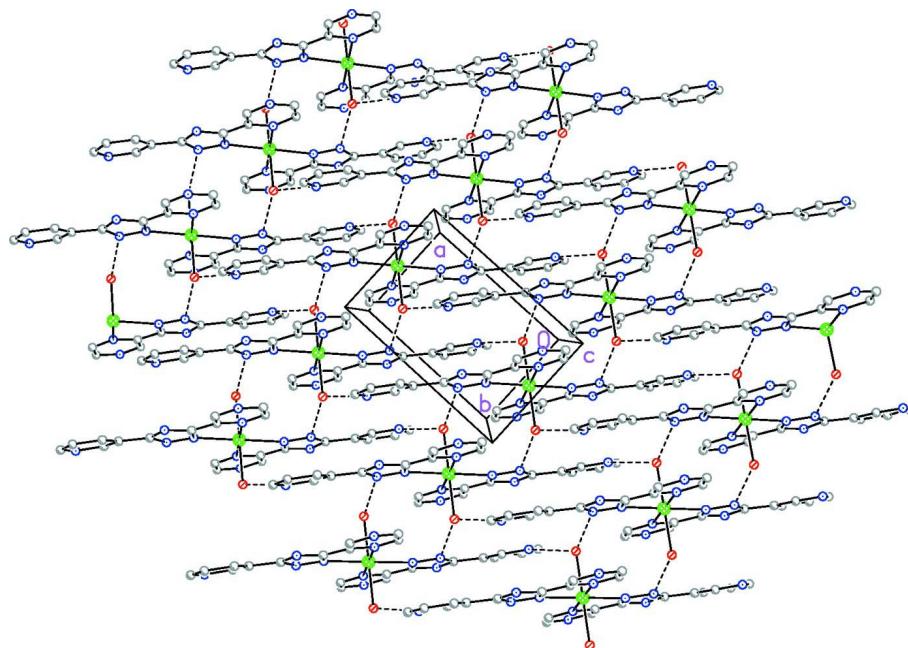
Figure 2

The two-dimensional network structure formed by hydrogen bonding interactions (dashed lines). H atoms are omitted for clarity.

Diaquabis[5-(pyrazin-2-yl-κN^1)-3-(pyridin-3-yl)-1,2,4- triazolido-κN^1]cadmium

Crystal data

[Cd(C$_{11}$H$_7$N$_6$)$_2$(H$_2$O)$_2$]	$b = 5.684$ (3) Å
$M_r = 594.88$	$c = 23.157$ (13) Å
Monoclinic, $P2_1/c$	$\beta = 99.102$ (6)°
Hall symbol: -P 2ybc	$V = 1122.9$ (11) Å^3
$a = 8.640$ (5) Å	$Z = 2$

$F(000) = 596$
$D_x = 1.759$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2671 reflections
$\theta = 2.4$–$27.5°$

$\mu = 1.02$ mm^{-1}
$T = 296$ K
Prism, colorless
$0.24 \times 0.21 \times 0.20$ mm

Data collection

Bruker SMART CCD
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.782$, $T_{max} = 0.815$

11387 measured reflections
2571 independent reflections
2251 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.081$
$S = 1.09$
2571 reflections
175 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 0.5415P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.0000	1.0000	0.0000	0.02997 (10)
N1	0.0416 (2)	1.1638 (3)	0.09658 (9)	0.0272 (4)
N2	0.0947 (3)	1.2756 (4)	0.21582 (9)	0.0365 (5)
N3	0.1919 (2)	0.7738 (3)	0.05584 (9)	0.0295 (4)
N4	0.2884 (2)	0.5850 (4)	0.05077 (9)	0.0306 (4)
N5	0.3260 (2)	0.6991 (3)	0.14563 (9)	0.0290 (4)
N6	0.6292 (3)	0.0309 (4)	0.09166 (12)	0.0395 (6)
O1	−0.1880 (2)	0.7608 (3)	0.03044 (8)	0.0343 (4)
H1A	−0.263 (3)	0.840 (5)	0.0406 (13)	0.051*
H1B	−0.227 (3)	0.657 (4)	0.0055 (12)	0.051*
C1	−0.0256 (3)	1.3500 (4)	0.11794 (11)	0.0321 (5)

H1	−0.0932	1.4440	0.0925	0.039*
C2	0.0024 (3)	1.4061 (5)	0.17639 (12)	0.0346 (6)
H2	−0.0445	1.5399	0.1890	0.042*
C3	0.1625 (3)	1.0904 (5)	0.19467 (11)	0.0340 (6)
H3	0.2281	0.9955	0.2206	0.041*
C4	0.1390 (3)	1.0333 (4)	0.13529 (11)	0.0257 (5)
C5	0.2188 (3)	0.8347 (4)	0.11250 (10)	0.0266 (5)
C6	0.3651 (3)	0.5483 (4)	0.10522 (12)	0.0272 (5)
C7	0.4792 (3)	0.3558 (4)	0.12057 (11)	0.0288 (5)
C8	0.5377 (3)	0.3073 (5)	0.17899 (12)	0.0343 (6)
H8	0.5079	0.3996	0.2085	0.041*
C9	0.6405 (3)	0.1208 (5)	0.19295 (12)	0.0379 (6)
H9	0.6810	0.0867	0.2317	0.045*
C10	0.6809 (3)	−0.0120 (4)	0.14809 (15)	0.0387 (7)
H10	0.7480	−0.1390	0.1576	0.046*
C11	0.5315 (3)	0.2144 (5)	0.07830 (12)	0.0361 (6)
H11	0.4972	0.2485	0.0391	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03525 (16)	0.03198 (15)	0.02068 (15)	0.00690 (10)	−0.00171 (11)	−0.00100 (9)
N1	0.0299 (10)	0.0262 (9)	0.0249 (10)	0.0034 (8)	0.0026 (8)	−0.0011 (8)
N2	0.0473 (13)	0.0357 (11)	0.0264 (11)	0.0039 (10)	0.0051 (10)	−0.0055 (9)
N3	0.0328 (10)	0.0286 (10)	0.0265 (11)	0.0071 (9)	0.0029 (8)	−0.0022 (8)
N4	0.0332 (11)	0.0292 (10)	0.0290 (11)	0.0085 (9)	0.0034 (9)	−0.0033 (9)
N5	0.0289 (10)	0.0302 (10)	0.0264 (10)	0.0061 (8)	0.0001 (8)	−0.0010 (8)
N6	0.0334 (12)	0.0420 (13)	0.0434 (15)	0.0122 (10)	0.0067 (11)	−0.0048 (10)
O1	0.0345 (9)	0.0326 (9)	0.0357 (10)	0.0041 (8)	0.0055 (8)	−0.0061 (8)
C1	0.0355 (13)	0.0287 (12)	0.0318 (13)	0.0068 (10)	0.0044 (11)	0.0012 (10)
C2	0.0423 (14)	0.0292 (12)	0.0342 (14)	0.0054 (11)	0.0119 (11)	−0.0028 (11)
C3	0.0411 (14)	0.0338 (13)	0.0251 (13)	0.0057 (11)	−0.0005 (11)	−0.0005 (11)
C4	0.0249 (11)	0.0282 (11)	0.0237 (12)	0.0012 (9)	0.0029 (9)	0.0017 (9)
C5	0.0262 (11)	0.0264 (11)	0.0269 (12)	0.0027 (9)	0.0036 (9)	−0.0001 (9)
C6	0.0237 (11)	0.0295 (11)	0.0281 (13)	0.0035 (9)	0.0033 (10)	−0.0002 (10)
C7	0.0256 (11)	0.0282 (11)	0.0316 (13)	0.0043 (9)	0.0018 (10)	0.0007 (10)
C8	0.0331 (13)	0.0359 (13)	0.0330 (14)	0.0057 (11)	0.0030 (11)	−0.0010 (11)
C9	0.0355 (14)	0.0410 (14)	0.0357 (15)	0.0077 (12)	0.0011 (11)	0.0070 (12)
C10	0.0323 (13)	0.0335 (14)	0.0497 (19)	0.0104 (11)	0.0045 (13)	0.0053 (11)
C11	0.0330 (13)	0.0431 (14)	0.0315 (14)	0.0084 (11)	0.0031 (11)	−0.0025 (11)

Geometric parameters (Å, º)

Cd1—O1[i]	2.312 (2)	O1—H1A	0.850 (17)
Cd1—O1	2.312 (2)	O1—H1B	0.859 (17)
Cd1—N1[i]	2.397 (2)	C1—C2	1.374 (4)
Cd1—N1	2.397 (2)	C1—H1	0.9300
Cd1—N3	2.323 (2)	C2—H2	0.9300

Cd1—N3ⁱ	2.323 (2)	C3—C4	1.396 (4)
N1—C1	1.339 (3)	C3—H3	0.9300
N1—C4	1.351 (3)	C4—C5	1.464 (3)
N2—C3	1.334 (3)	C6—C7	1.478 (3)
N2—C2	1.338 (3)	C7—C11	1.396 (4)
N3—C5	1.341 (3)	C7—C8	1.395 (4)
N3—N4	1.375 (3)	C8—C9	1.388 (4)
N4—C6	1.345 (3)	C8—H8	0.9300
N5—C5	1.347 (3)	C9—C10	1.373 (4)
N5—C6	1.351 (3)	C9—H9	0.9300
N6—C10	1.335 (4)	C10—H10	0.9300
N6—C11	1.347 (3)	C11—H11	0.9300
O1ⁱ—Cd1—O1	180.00 (9)	N2—C2—C1	122.4 (2)
O1ⁱ—Cd1—N3	91.20 (8)	N2—C2—H2	118.8
O1—Cd1—N3	88.80 (8)	C1—C2—H2	118.8
O1ⁱ—Cd1—N3ⁱ	88.80 (8)	N2—C3—C4	122.8 (2)
O1—Cd1—N3ⁱ	91.20 (8)	N2—C3—H3	118.6
N3—Cd1—N3ⁱ	180.00 (9)	C4—C3—H3	118.6
O1ⁱ—Cd1—N1ⁱ	87.30 (7)	N1—C4—C3	120.3 (2)
O1—Cd1—N1ⁱ	92.70 (7)	N1—C4—C5	117.6 (2)
N3—Cd1—N1ⁱ	107.04 (7)	C3—C4—C5	122.1 (2)
N3ⁱ—Cd1—N1ⁱ	72.96 (7)	N3—C5—N5	114.0 (2)
O1ⁱ—Cd1—N1	92.70 (7)	N3—C5—C4	122.2 (2)
O1—Cd1—N1	87.30 (7)	N5—C5—C4	123.8 (2)
N3—Cd1—N1	72.96 (7)	N4—C6—N5	114.3 (2)
N3ⁱ—Cd1—N1	107.04 (7)	N4—C6—C7	123.5 (2)
N1ⁱ—Cd1—N1	180.00 (4)	N5—C6—C7	122.2 (2)
C1—N1—C4	116.8 (2)	C11—C7—C8	117.3 (2)
C1—N1—Cd1	129.95 (16)	C11—C7—C6	122.3 (2)
C4—N1—Cd1	113.06 (15)	C8—C7—C6	120.4 (2)
C3—N2—C2	115.8 (2)	C9—C8—C7	119.8 (2)
C5—N3—N4	105.73 (19)	C9—C8—H8	120.1
C5—N3—Cd1	113.59 (15)	C7—C8—H8	120.1
N4—N3—Cd1	140.64 (16)	C10—C9—C8	118.3 (3)
C6—N4—N3	104.86 (19)	C10—C9—H9	120.9
C5—N5—C6	101.1 (2)	C8—C9—H9	120.9
C10—N6—C11	117.8 (2)	N6—C10—C9	123.7 (2)
Cd1—O1—H1A	112 (2)	N6—C10—H10	118.2
Cd1—O1—H1B	115 (2)	C9—C10—H10	118.2
H1A—O1—H1B	108 (2)	N6—C11—C7	123.1 (3)
N1—C1—C2	121.9 (2)	N6—C11—H11	118.5
N1—C1—H1	119.1	C7—C11—H11	118.5
C2—C1—H1	119.1		
O1ⁱ—Cd1—N1—C1	88.8 (2)	Cd1—N1—C4—C5	7.6 (3)
O1—Cd1—N1—C1	−91.2 (2)	N2—C3—C4—N1	−1.6 (4)
N3—Cd1—N1—C1	179.3 (2)	N2—C3—C4—C5	177.7 (2)

N3^i—Cd1—N1—C1	−0.7 (2)	N4—N3—C5—N5	−0.3 (3)
N1^i—Cd1—N1—C1	−49.9 (6)	Cd1—N3—C5—N5	177.79 (16)
O1^i—Cd1—N1—C4	−97.06 (17)	N4—N3—C5—C4	179.0 (2)
O1—Cd1—N1—C4	82.94 (17)	Cd1—N3—C5—C4	−2.9 (3)
N3—Cd1—N1—C4	−6.62 (16)	C6—N5—C5—N3	0.3 (3)
N3^i—Cd1—N1—C4	173.38 (16)	C6—N5—C5—C4	−179.0 (2)
N1^i—Cd1—N1—C4	124.2 (4)	N1—C4—C5—N3	−3.4 (3)
O1^i—Cd1—N3—C5	97.31 (17)	C3—C4—C5—N3	177.4 (2)
O1—Cd1—N3—C5	−82.69 (17)	N1—C4—C5—N5	175.8 (2)
N3^i—Cd1—N3—C5	−54 (63)	C3—C4—C5—N5	−3.5 (4)
N1^i—Cd1—N3—C5	−175.14 (16)	N3—N4—C6—N5	0.0 (3)
N1—Cd1—N3—C5	4.86 (16)	N3—N4—C6—C7	178.2 (2)
O1^i—Cd1—N3—N4	−85.7 (3)	C5—N5—C6—N4	−0.2 (3)
O1—Cd1—N3—N4	94.3 (3)	C5—N5—C6—C7	−178.4 (2)
N3^i—Cd1—N3—N4	123 (62)	N4—C6—C7—C11	8.4 (4)
N1^i—Cd1—N3—N4	1.9 (3)	N5—C6—C7—C11	−173.5 (2)
N1—Cd1—N3—N4	−178.1 (3)	N4—C6—C7—C8	−170.8 (2)
C5—N3—N4—C6	0.1 (3)	N5—C6—C7—C8	7.2 (4)
Cd1—N3—N4—C6	−177.05 (19)	C11—C7—C8—C9	−1.5 (4)
C4—N1—C1—C2	−0.1 (4)	C6—C7—C8—C9	177.7 (2)
Cd1—N1—C1—C2	173.81 (19)	C7—C8—C9—C10	−0.4 (4)
C3—N2—C2—C1	2.1 (4)	C11—N6—C10—C9	−0.3 (4)
N1—C1—C2—N2	−1.9 (4)	C8—C9—C10—N6	1.3 (4)
C2—N2—C3—C4	−0.4 (4)	C10—N6—C11—C7	−1.8 (4)
C1—N1—C4—C3	1.8 (3)	C8—C7—C11—N6	2.7 (4)
Cd1—N1—C4—C3	−173.18 (19)	C6—C7—C11—N6	−176.5 (2)
C1—N1—C4—C5	−177.5 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N6^{ii}	0.85 (2)	1.95 (2)	2.751 (3)	157 (3)
O1—H1*B*···N4^{iii}	0.86 (2)	1.91 (2)	2.763 (3)	173 (3)

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