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Bis(μ-5-carboxylatotetrazolido)bis[aqua(2,2′-bipyridyl)cadmium(II)]

Shuang-Jiao Sun,[a]* Ji-Hua Deng[b] and Ti-Lou Liu[a]

[a]Shaoyang Medical College, Shaoyang, Hunan 422000, People's Republic of China, and [b]College of Chemistry and Bio-engineering, Yichun University, Yichun, Jiangxi 336000, People's Republic of China
Correspondence e-mail: sshj_2008@yahoo.cn

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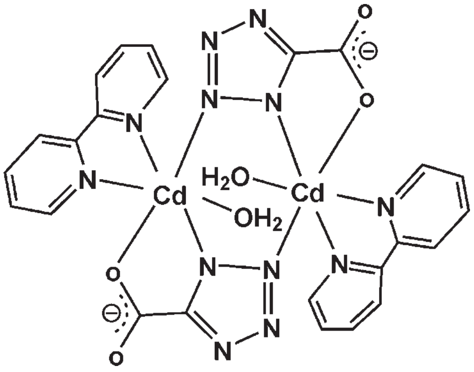
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.025; wR factor = 0.066; data-to-parameter ratio = 10.5.

In the title dinuclear Cd^{II} complex, $[Cd_2(C_2N_4O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$, each Cd atom is in a slightly distorted octahedral coordination by two N atoms and one O atom of two 1*H*-tetrazole-5-carboxylate (TZC) ligands, two N atoms of a 2,2′-bipyridyl ligand and one water O atom. The TZC ligand acts in a tridentate *N*,*O*-chelating *N*-bridging mode to two symmetry-equivalent Cd^{II} atoms. The complex reveals molecular C_i symmetry. Extensive O—H⋯O hydrogen bonding plays an important role in the crystal packing.

Related literature

For the structural topologies and varied properties such as molecular magnetism, molecular absorption, catalysis, non-linear optics and luminescence of coordination complexes with tetrazolate-based ligands, see: Zhao *et al.* (2008); Cheng *et al.* (2007). For related structures, see: Wu *et al.* (2009; 2010) For related literature on 1*H*-tetrazoles, see: Jia *et al.* (2009); Zhong *et al.* (2010).



Experimental

Crystal data

$[Cd_2(C_2N_4O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 797.32
Triclinic, $P\overline{1}$
a = 7.5218 (13) Å
b = 9.6372 (16) Å
c = 9.7335 (16) Å
α = 75.628 (3)°
β = 89.686 (3)°
γ = 74.461 (2)°
V = 657.10 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 173 K
0.28 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.650, T_{max} = 0.774
3760 measured reflections
2168 independent reflections
1930 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.066
S = 1.11
2168 reflections
207 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—N9	2.285 (3)	Cd1—O3	2.314 (3)
Cd1—N2^{i}	2.304 (3)	Cd1—O1	2.330 (2)
Cd1—N1	2.310 (3)	Cd1—N10	2.352 (3)

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H3*B*⋯O2^{ii}	0.83 (2)	2.01 (3)	2.794 (4)	158 (4)
O3—H3*A*⋯O2^{iii}	0.80 (2)	2.09 (4)	2.769 (4)	143 (4)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2269).

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m982 Sun *et al.* • $[Cd_2(C_2N_4O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$ *Acta Cryst.* (2010). E**66**, m981–m982

supporting information

Acta Cryst. (2010). E**66**, m981–m982   [https://doi.org/10.1107/S1600536810027613]

Bis(μ-5-carboxylatotetrazolido)bis[aqua(2,2′-bipyridyl)cadmium(II)]

Shuang-Jiao Sun, Ji-Hua Deng and Ti-Lou Liu

S1. Comment

Coordination complexes with tetrazolate-based ligands have been the subject of intense research efforts in recent years, owing to their enormous variety of interesting structural topologies, and wide physical properties such as molecular magnetism, molecular absorption, catalysis, non-linear optics, and luminescence (Zhao, 2008; Cheng *et al.*, 2007). The crystal structures and properties of metal complexes based on tetrazolate-5-carboxylato ligand have been reported in several papers (Wu *et al.*, 2009; Wu *et al.*, 2010) in recent years. Herein, we report the synthesis and crystal structure of its cadmium(II) complex.

In the title compound (I), the asymmetric unit comprises a half of the molecule (Fig. 1) and an inversion symmetry generates a dinuclear complex. The bond lengths (Table 1) and angles around Cd1 atom suggests a slightly distorted octahedral geometry. The TZC ligand acts as a tridentate linker to chelate the Cd atom and bridges the other Cd atom in a μ_2-N2:O1,N1 coordination mode (Fig. 1). Two Cd atoms are bridged by tetrazolate groups from two symmetry-related TZC ligands to form one six-membered ring (Cd1—N1—N2—Cd1A—N1A—N2A). There are O–H···O, C–H···N, C–H···O intermolecular hydrogen bonds (Table 2). The molecules are held together by intermolecular hydrogen bonding interactions, forming a three-dimensional network (Fig. 2).

S2. Experimental

A mixture of $Cd(NO_3)_2\ 4H_2O$ (0.5 mmol), TZC (0.5 mmol), KOH (0.5 mmol) and 2,2′-bipy (0.5 mmol) in aqueous solution (15 ml) was sealed in a 25 ml Teflon-lined stainless steel vessel under autogenous pressure and heated at 383 K for 3 days, and then slowly cooled to room temperature. Colourless crystals suitable for X-ray analyses were obtained, washed with distilled water and dried in air. Yield: 50% (based on Cd).

S3. Refinement

The H atoms of the 2,2′-bipy were placed in geometrically idealized positions with C—H distances of 0.93 Å, and were refined isotropic using a riding model with U_{iso}(H) = 1.2Ueq(C). The H atoms of the coordinated water molecules were assigned in the difference Fourier maps and refined isotropically.

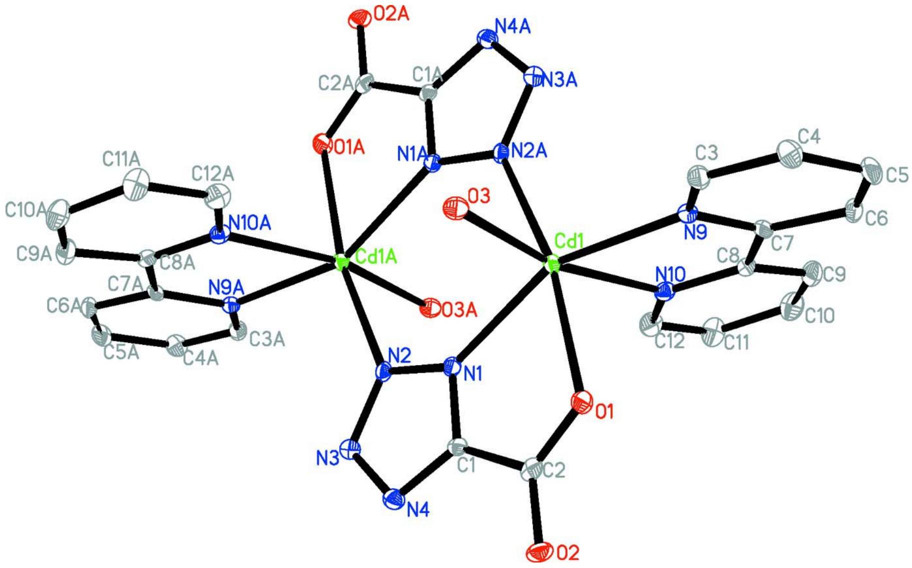

Figure 1

The structure of (**I**), showing 30% probability displacement ellipsoids and the atom-labeling scheme. Symmetry code: (A) -*x* + 1, -*y*, -*z* + 1.

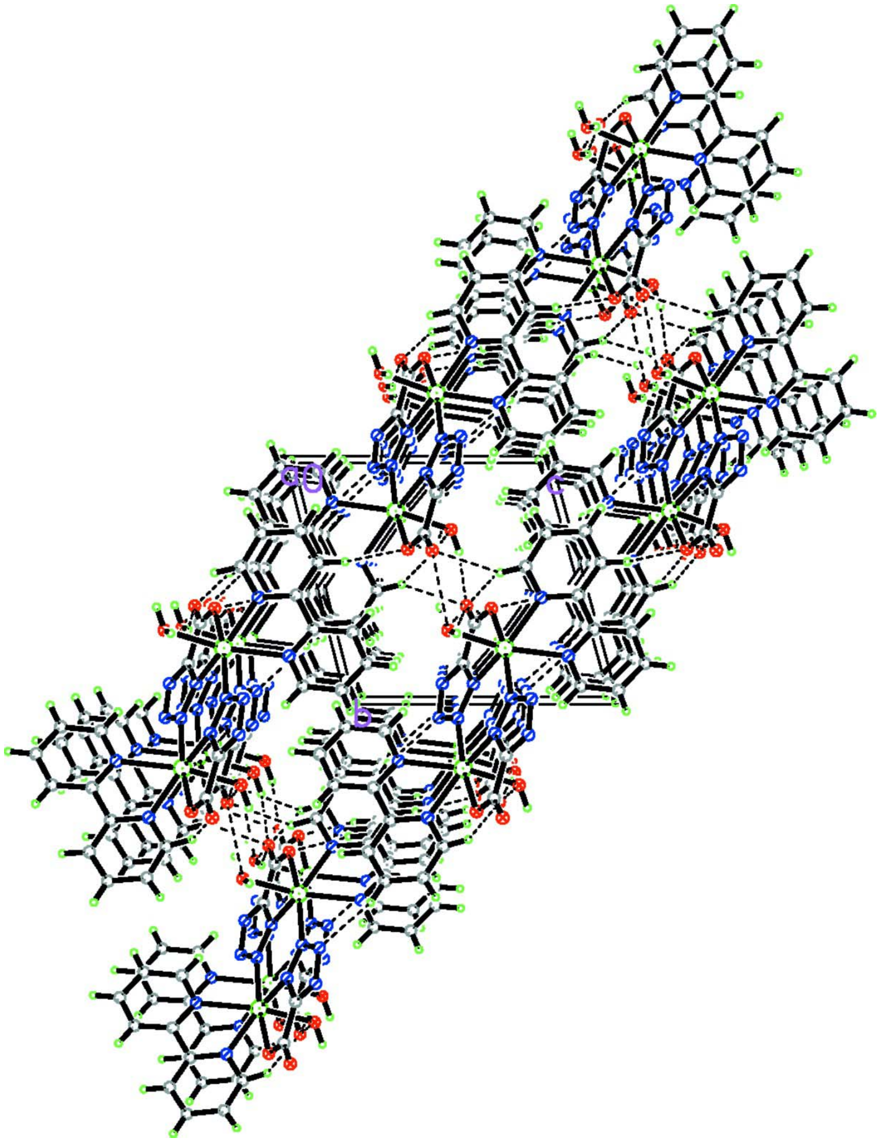

Figure 2

Three-dimensional network of hydrogen bonds.

Bis(μ-5-carboxylatotetrazolido)bis[aqua(2,2′-bipyridyl)cadmium(II)]

Crystal data

$[Cd_2(C_2N_4O_2)_2(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 797.32
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.5218 (13) Å
b = 9.6372 (16) Å
c = 9.7335 (16) Å
α = 75.628 (3)°
β = 89.686 (3)°
γ = 74.461 (2)°
V = 657.10 (19) Å^3

Z = 1
F(000) = 392
D_x = 2.015 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2926 reflections
θ = 2.7–27.0°
μ = 1.69 mm^{-1}
T = 173 K
Block, colourless
0.28 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3760 measured reflections
Radiation source: fine-focus sealed tube	2268 independent reflections
Graphite monochromator	1930 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{\mathrm{int}} = 0.019$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	$\theta_{\mathrm{max}} = 25.0°$, $\theta_{\mathrm{min}} = 2.2°$
$T_{\mathrm{min}} = 0.650$, $T_{\mathrm{max}} = 0.774$	$h = -8 \rightarrow 8$
	$k = -11 \rightarrow 11$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.066$	$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.4626P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{\mathrm{max}} < 0.001$
2168 reflections	$\Delta\rho_{\mathrm{max}} = 0.70$ e Å^{-3}
207 parameters	$\Delta\rho_{\mathrm{min}} = -0.47$ e Å^{-3}
3 restraints	
Primary atom site location: structure-invariant direct methods	

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	0.40965 (3)	0.23221 (3)	0.36929 (3)	0.01494 (11)
O1	0.6019 (3)	0.3838 (3)	0.3780 (3)	0.0205 (6)
O2	0.8715 (3)	0.3914 (3)	0.4648 (3)	0.0212 (6)
O3	0.2432 (3)	0.3036 (3)	0.5528 (3)	0.0199 (6)
N1	0.6687 (4)	0.0890 (3)	0.5152 (3)	0.0145 (6)
N2	0.7360 (4)	−0.0460 (3)	0.6050 (3)	0.0150 (6)
N3	0.8896 (4)	−0.0486 (4)	0.6726 (3)	0.0187 (7)
N4	0.9234 (4)	0.0835 (3)	0.6289 (3)	0.0181 (7)
N9	0.2429 (4)	0.4286 (3)	0.1938 (3)	0.0151 (6)
N10	0.5150 (4)	0.1995 (3)	0.1484 (3)	0.0167 (7)
C1	0.7862 (5)	0.1654 (4)	0.5330 (4)	0.0142 (8)
C2	0.7527 (5)	0.3265 (4)	0.4521 (4)	0.0174 (8)
C3	0.1195 (5)	0.5462 (4)	0.2218 (4)	0.0190 (8)
H3	0.0696	0.5230	0.3173	0.023*
C4	0.0345 (5)	0.6728 (4)	0.1188 (4)	0.0230 (9)

H4	−0.0526	0.7532	0.1432	0.028*
C5	0.0777 (5)	0.6817 (4)	−0.0214 (4)	0.0232 (9)
H5	0.0196	0.7672	−0.0951	0.028*
C6	0.2080 (5)	0.5619 (4)	−0.0508 (4)	0.0189 (8)
H6	0.2427	0.5655	−0.1454	0.023*
C7	0.2875 (5)	0.4368 (4)	0.0589 (4)	0.0156 (8)
C8	0.4293 (5)	0.3049 (4)	0.0329 (4)	0.0157 (8)
C9	0.4693 (5)	0.2928 (5)	−0.1038 (4)	0.0240 (9)
H9	0.4056	0.3679	−0.1842	0.029*
C10	0.6035 (6)	0.1695 (5)	−0.1209 (4)	0.0289 (10)
H10	0.6316	0.1582	−0.2134	0.035*
C11	0.6960 (6)	0.0634 (5)	−0.0029 (4)	0.0282 (9)
H11	0.7911	−0.0205	−0.0128	0.034*
C12	0.6479 (5)	0.0810 (4)	0.1307 (4)	0.0243 (9)
H12	0.7106	0.0072	0.2123	0.029*
H3A	0.149 (5)	0.288 (5)	0.531 (5)	0.037 (14)*
H3B	0.234 (6)	0.388 (4)	0.563 (5)	0.045 (15)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01564 (15)	0.01420 (16)	0.01338 (16)	−0.00440 (11)	−0.00143 (10)	−0.00027 (11)
O1	0.0236 (14)	0.0146 (13)	0.0214 (14)	−0.0080 (11)	−0.0036 (11)	0.0020 (11)
O2	0.0216 (13)	0.0211 (14)	0.0258 (15)	−0.0135 (12)	0.0028 (11)	−0.0069 (12)
O3	0.0193 (14)	0.0196 (15)	0.0226 (15)	−0.0068 (12)	0.0009 (11)	−0.0071 (12)
N1	0.0158 (15)	0.0149 (16)	0.0129 (16)	−0.0050 (13)	0.0013 (12)	−0.0028 (13)
N2	0.0163 (15)	0.0139 (16)	0.0122 (16)	−0.0035 (13)	0.0010 (12)	0.0008 (13)
N3	0.0174 (15)	0.0203 (17)	0.0183 (17)	−0.0062 (14)	0.0006 (13)	−0.0037 (14)
N4	0.0158 (15)	0.0193 (17)	0.0186 (17)	−0.0039 (13)	0.0000 (13)	−0.0048 (14)
N9	0.0146 (14)	0.0157 (16)	0.0154 (16)	−0.0054 (13)	0.0004 (12)	−0.0035 (13)
N10	0.0159 (15)	0.0134 (16)	0.0204 (17)	−0.0047 (13)	0.0021 (13)	−0.0027 (13)
C1	0.0130 (16)	0.019 (2)	0.0132 (18)	−0.0056 (15)	0.0047 (14)	−0.0077 (16)
C2	0.0219 (19)	0.022 (2)	0.0133 (19)	−0.0091 (17)	0.0087 (16)	−0.0108 (16)
C3	0.0181 (18)	0.020 (2)	0.017 (2)	−0.0035 (16)	0.0011 (16)	−0.0034 (16)
C4	0.0218 (19)	0.018 (2)	0.025 (2)	−0.0004 (17)	−0.0010 (17)	−0.0043 (17)
C5	0.0231 (19)	0.017 (2)	0.023 (2)	−0.0026 (17)	−0.0066 (17)	0.0033 (17)
C6	0.0233 (19)	0.020 (2)	0.0126 (19)	−0.0088 (17)	0.0002 (16)	0.0000 (16)
C7	0.0150 (17)	0.0170 (19)	0.0151 (19)	−0.0071 (15)	−0.0031 (15)	−0.0018 (16)
C8	0.0146 (17)	0.0166 (19)	0.0159 (19)	−0.0058 (15)	0.0015 (15)	−0.0027 (16)
C9	0.028 (2)	0.027 (2)	0.017 (2)	−0.0085 (18)	0.0041 (17)	−0.0045 (17)
C10	0.034 (2)	0.031 (2)	0.022 (2)	−0.007 (2)	0.0113 (19)	−0.0107 (19)
C11	0.033 (2)	0.018 (2)	0.029 (2)	−0.0001 (18)	0.0075 (19)	−0.0059 (18)
C12	0.024 (2)	0.016 (2)	0.029 (2)	−0.0026 (17)	0.0019 (17)	−0.0024 (17)

Geometric parameters (Å, º)

Cd1—N9	2.285 (3)	N10—C12	1.349 (5)
Cd1—N2^{i}	2.304 (3)	C1—C2	1.510 (5)

Cd1—N1	2.310 (3)	C3—C4	1.372 (5)
Cd1—O3	2.314 (3)	C3—H3	0.9966
Cd1—O1	2.330 (2)	C4—C5	1.388 (6)
Cd1—N10	2.352 (3)	C4—H4	0.9500
O1—C2	1.260 (4)	C5—C6	1.389 (5)
O2—C2	1.242 (4)	C5—H5	0.9500
O3—H3A	0.80 (2)	C6—C7	1.390 (5)
O3—H3B	0.83 (2)	C6—H6	0.9500
N1—C1	1.329 (5)	C7—C8	1.500 (5)
N1—N2	1.342 (4)	C8—C9	1.389 (5)
N2—N3	1.324 (4)	C9—C10	1.382 (5)
N2—Cd1^{i}	2.304 (3)	C9—H9	0.9500
N3—N4	1.330 (4)	C10—C11	1.376 (6)
N4—C1	1.330 (5)	C10—H10	0.9500
N9—C7	1.342 (5)	C11—C12	1.386 (6)
N9—C3	1.344 (5)	C11—H11	0.9500
N10—C8	1.342 (5)	C12—H12	0.9500

N9—Cd1—N2^{i}	106.72 (10)	N4—C1—C2	127.8 (3)
N9—Cd1—N1	155.62 (10)	O2—C2—O1	125.7 (4)
N2^{i}—Cd1—N1	96.01 (10)	O2—C2—C1	118.7 (3)
N9—Cd1—O3	95.41 (10)	O1—C2—C1	115.6 (3)
N2^{i}—Cd1—O3	87.65 (10)	N9—C3—C4	123.2 (3)
N1—Cd1—O3	94.18 (9)	N9—C3—H3	113.3
N9—Cd1—O1	85.09 (10)	C4—C3—H3	121.4
N2^{i}—Cd1—O1	168.16 (9)	C3—C4—C5	119.0 (4)
N1—Cd1—O1	72.19 (10)	C3—C4—H4	120.5
O3—Cd1—O1	92.14 (9)	C5—C4—H4	120.5
N9—Cd1—N10	71.32 (10)	C4—C5—C6	118.2 (4)
N2^{i}—Cd1—N10	91.88 (10)	C4—C5—H5	120.9
N1—Cd1—N10	99.78 (10)	C6—C5—H5	120.9
O3—Cd1—N10	166.00 (10)	C5—C6—C7	119.6 (3)
O1—Cd1—N10	91.16 (10)	C5—C6—H6	120.2
C2—O1—Cd1	118.0 (2)	C7—C6—H6	120.2
Cd1—O3—H3A	96 (3)	N9—C7—C6	121.7 (3)
Cd1—O3—H3B	119 (3)	N9—C7—C8	116.5 (3)
H3A—O3—H3B	117 (3)	C6—C7—C8	121.7 (3)
C1—N1—N2	104.9 (3)	N10—C8—C9	121.9 (3)
C1—N1—Cd1	113.4 (2)	N10—C8—C7	116.5 (3)
N2—N1—Cd1	141.1 (2)	C9—C8—C7	121.5 (3)
N3—N2—N1	108.9 (3)	C10—C9—C8	118.8 (4)
N3—N2—Cd1^{i}	128.6 (2)	C10—C9—H9	120.6
N1—N2—Cd1^{i}	122.5 (2)	C8—C9—H9	120.6
N2—N3—N4	109.4 (3)	C11—C10—C9	119.5 (4)
N3—N4—C1	105.2 (3)	C11—C10—H10	120.2
C7—N9—C3	118.2 (3)	C9—C10—H10	120.2
C7—N9—Cd1	118.7 (2)	C10—C11—C12	118.8 (4)
C3—N9—Cd1	122.4 (2)	C10—C11—H11	120.6

C8—N10—C12	118.8 (3)	C12—C11—H11	120.6
C8—N10—Cd1	116.4 (2)	N10—C12—C11	122.1 (4)
C12—N10—Cd1	124.7 (3)	N10—C12—H12	119.0
N1—C1—N4	111.6 (3)	C11—C12—H12	119.0
N1—C1—C2	120.6 (3)		

Symmetry code: (i) −*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$^{\mathrm{ii}}$	0.83 (2)	2.01 (3)	2.794 (4)	158 (4)
O3—H3*A*···O2$^{\mathrm{iii}}$	0.80 (2)	2.09 (4)	2.769 (4)	143 (4)

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