Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

The one-dimensional polymer poly[[aqua(2,2′-bipyridine)cadmium(II)]-*μ*-*trans*-stilbene-4,4′-dicarboxylato]

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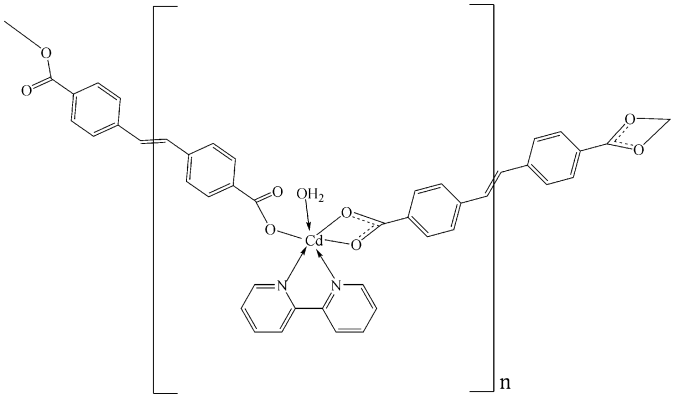
Received 11 November 2007; accepted 3 December 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.073; data-to-parameter ratio = 16.1.

In the title polymer, $[Cd(C_{16}H_{10}O_4)(C_{10}H_8N_2)(H_2O)]_n$, the Cd^{II} ion is in a strongly distorted octahedral geometry, being coordinated by two N atoms from a 2,2′-bipyridine ligand, three carboxylate O atoms from two symmetry-related *trans*-stilbene-4,4′-dicarboxylate dianions and one water molecule. The stilbene ligand lies on an inversion centre at the midpoint of the central C=C bond. This feature generates the polymeric structure: adjacent Cd^{II} ions are bridged by *trans*-stilbene-4,4′-dicarboxylate dianions, giving rise to a one-dimensional structure. The coordinated water molecule is involved in interchain O—H···O hydrogen bonds.

Related literature

A closely related Ni^{II} complex with 1,10-phenanthroline and the *trans*-stilbene-4,4′-dicarboxylate dianion as ligands has been characterized by X-ray diffraction (Wang *et al.*, 2006).



Experimental

Crystal data

$[Cd(C_{16}H_{10}O_4)(C_{10}H_8N_2)(H_2O)]$
M_r = 552.84
Triclinic, $P\overline{1}$
a = 10.543 (2) Å
b = 10.838 (2) Å
c = 11.442 (2) Å
α = 98.90 (3)°
β = 115.07 (3)°
γ = 102.95 (3)°
V = 1107.0 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 295 (2) K
0.35 × 0.26 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.715, T_{max} = 0.861
10929 measured reflections
5024 independent reflections
4482 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.073
S = 1.08
5024 reflections
313 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O2	2.209 (2)	Cd1—O1*W*	2.291 (2)
Cd1—O1	2.745 (2)	Cd1—N1	2.316 (3)
Cd1—O3	2.2129 (19)	Cd1—N2	2.375 (2)
O1—Cd1—O1*W*	139.33 (8)	O2—Cd1—N1	144.70 (8)
O1—Cd1—O2	51.29 (8)	O3—Cd1—N1	87.35 (8)
O1—Cd1—O3	120.67 (8)	O1*W*—Cd1—N1	112.58 (8)
O1—Cd1—N1	94.47 (8)	O2—Cd1—N2	89.94 (8)
O1—Cd1—N2	74.71 (8)	O3—Cd1—N2	154.30 (8)
O2—Cd1—O3	115.76 (8)	O1*W*—Cd1—N2	86.30 (8)
O2—Cd1—O1*W*	94.06 (8)	N1—Cd1—N2	70.07 (8)
O3—Cd1—O1*W*	91.48 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{i}	0.850 (10)	1.918 (18)	2.697 (3)	152 (3)
O1*W*—H1*W*2···O4^{i}	0.85 (4)	1.81 (4)	2.639 (3)	167 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

We thank the Heilongjiang Province Natural Science Foundation (No. B200501) and the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036), Heilongjiang University, for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2152).

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Wang, H.-Y., Gao, S., Huo, L.-H. & Zhao, J.-G. (2006). *Acta Cryst.* E**62**, m3395–m3397.

supporting information

Acta Cryst. (2008). E**64**, m162–m163 [https://doi.org/10.1107/S1600536807065294]

The one-dimensional polymer poly[[aqua(2,2′-bipyridine)cadmium(II)]-*μ*-*trans*-stilbene-4,4′-dicarboxylato]

Huan-Yu Wang, Shan Gao, Li-Hua Huo and Jing-Gui Zhao

S1. Comment

We are interested in the solid-state coordination chemistry of *trans*-stilbene-4,4′-dicarboxylic acid, combined with specific transition metal ions, to fabricate versatile coordination polymers. In our previous work, a one-dimensional Ni^{II}-organic framework had been reported (Wang *et al.*, 2006). In order to further explore the behavior of *trans*-stilbene-4,4′-dicarboxylic acid as ligand, a new one-dimensional Cd^{II} complex has been obtained and characterized.

The molecular structure of the title compound is illustrated in Fig. 1. The Cd^{II} ion is in a strongly distorted octahedral geometry and is coordinated by two N atoms of a 2,2′-bipyridine ligand, three carboxyl O atoms of two symmetry-related *trans*-stilbene-4,4′-dicarboxylato dianions, which adopted two different coordination modes, and one water molecule. One of the two carboxylic ligands is found in the bis-monodentate mode, and the other in the chelating bis-bidentate mode, linking the adjacent Cd^{II} ions into a zigzag chain structure. In addition, the chains are interconnected through intermolecular hydrogen bonds involving water molecules, and *π*–*π* interactions involving 2,2′-bipyridine ligands, [centroid-to-centroid separation: 3.8749 (10) Å], forming a three-dimensional supramolecular network (Table 2 and Fig. 2).

S2. Experimental

A mixture of $CdCl_2.6H_2O$ (1 mmol), 2,2′-bipyridine (1 mmol), *trans*-stilbene-4,4′-dicarboxylic acid (1 mmol) and water (10 ml) was stirred for 15 min. in air, then transferred and sealed in a 23 ml Parr teflon-lined stainless steel vessel, heated to 433 K for 5 days, and then cooled to room temperature. The resulting colorrless crystals were filtered, washed, and dried in air. Analysis calculated for $C_{26}H_{20}CdN_2O_5$: C 56.31, H 3.64, N 5.05%; found: C 56.34, H 3.62, N 5.03%.

S3. Refinement

Water H atoms were located in a difference map and refined with O—H and H···H distances restrained to 0.85 (1) and 1.39 (1) Å, respectively, and U_{iso}(H) = 1.5U_{eq}(O1W). All other H atoms were placed in calculated positions with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier C), and were refined in the riding-model approximation.

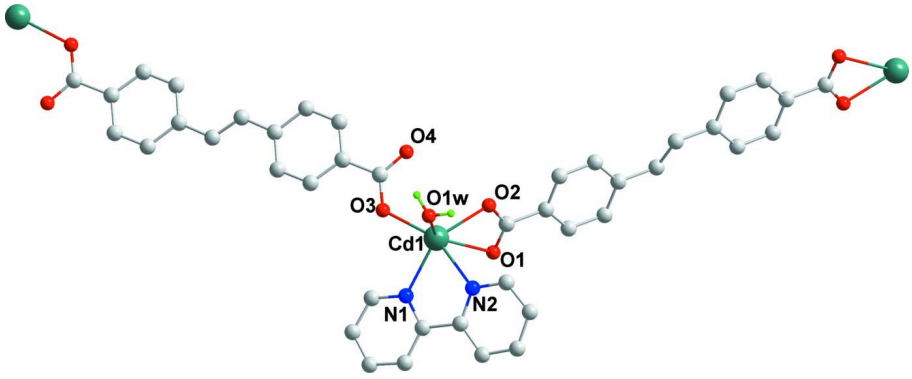

Figure 1

The molecular structure of the title complex. C-bonded H atoms have been omitted for clarity.

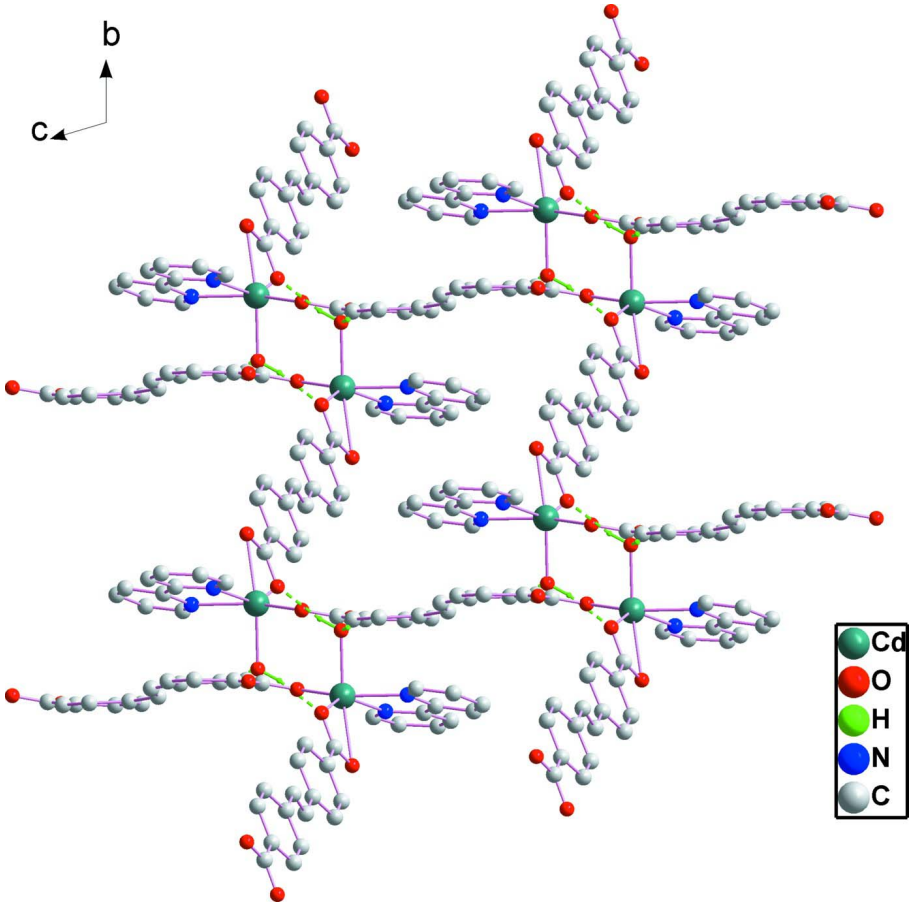

Figure 2

The packing diagram of the title complex, with the intermolecular hydrogen bonds denoted by dashed lines.

Poly[[aqua(2,2′-bipyridine)cadmium(II)]- *μ-trans*-stilbene-4,4′-dicarboxylato]

Crystal data

$[Cd(C_{16}H_{10}O_4)(C_{10}H_8N_2)(H_2O)]$
M_r = 552.84
Triclinic, $P\overline{1}$

Hall symbol: -P 1
a = 10.543 (2) Å
b = 10.838 (2) Å

c = 11.442 (2) Å
α = 98.90 (3)°
β = 115.07 (3)°
γ = 102.95 (3)°
V = 1107.0 (6) Å^3
Z = 2
F(000) = 556
D_x = 1.659 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9882 reflections
θ = 3.1–27.5°
μ = 1.03 mm^{-1}
T = 295 K
Block, colourless
0.35 × 0.26 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.715, T_{max} = 0.861

10929 measured reflections
5024 independent reflections
4482 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −13→13
k = −14→14
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.073
S = 1.08
5024 reflections
313 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
$w = 1/[\sigma^2(F_o^2) + (0.0341P)^2 + 0.8869P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.250536 (19)	0.691211 (19)	0.648737 (17)	0.02976 (7)
O1	0.1953 (2)	0.9264 (2)	0.6820 (2)	0.0420 (5)
O1W	0.1557 (2)	0.4774 (2)	0.6441 (2)	0.0375 (4)
H1W2	0.088 (3)	0.475 (3)	0.666 (3)	0.056*
H1W1	0.121 (3)	0.419 (3)	0.570 (2)	0.056*
O2	0.0352 (2)	0.7264 (2)	0.5764 (2)	0.0448 (5)
O3	0.3107 (2)	0.6262 (2)	0.49176 (19)	0.0474 (5)
O4	0.0819 (3)	0.5544 (3)	0.3238 (2)	0.0666 (7)
N1	0.5016 (2)	0.7824 (2)	0.7968 (2)	0.0334 (5)
N2	0.2902 (2)	0.7500 (2)	0.8731 (2)	0.0339 (5)
C1	0.6036 (3)	0.7890 (3)	0.7554 (3)	0.0420 (6)
H1	0.5719	0.7596	0.6637	0.050*
C2	0.7535 (3)	0.8376 (3)	0.8427 (3)	0.0502 (8)
H2	0.8218	0.8411	0.8110	0.060*
C3	0.7991 (3)	0.8808 (4)	0.9778 (3)	0.0539 (8)
H3	0.8995	0.9138	1.0393	0.065*
C4	0.6959 (3)	0.8750 (3)	1.0219 (3)	0.0455 (7)

H4	0.7261	0.9051	1.1132	0.055*
C5	0.5465 (3)	0.8241 (2)	0.9295 (2)	0.0315 (5)
C6	0.4290 (3)	0.8130 (2)	0.9701 (2)	0.0307 (5)
C7	0.4608 (4)	0.8664 (3)	1.1016 (3)	0.0436 (7)
H7	0.5579	0.9100	1.1685	0.052*
C8	0.3456 (4)	0.8533 (3)	1.1311 (3)	0.0510 (8)
H8	0.3646	0.8883	1.2186	0.061*
C9	0.2027 (4)	0.7887 (3)	1.0315 (3)	0.0483 (7)
H9	0.1238	0.7791	1.0498	0.058*
C10	0.1799 (3)	0.7382 (3)	0.9030 (3)	0.0413 (6)
H10	0.0835	0.6942	0.8347	0.050*
C11	0.0672 (3)	0.8507 (3)	0.6204 (2)	0.0333 (5)
C12	−0.0621 (3)	0.8999 (3)	0.5960 (2)	0.0313 (5)
C13	−0.2056 (3)	0.8142 (3)	0.5195 (3)	0.0434 (7)
H13	−0.2220	0.7254	0.4846	0.052*
C14	−0.3248 (3)	0.8590 (3)	0.4943 (3)	0.0426 (7)
H15	−0.4204	0.8000	0.4418	0.051*
C15	−0.3044 (3)	0.9907 (3)	0.5460 (3)	0.0307 (5)
C16	−0.1598 (3)	1.0773 (3)	0.6219 (3)	0.0350 (6)
H16	−0.1433	1.1661	0.6574	0.042*
C17	−0.0405 (3)	1.0325 (3)	0.6451 (3)	0.0340 (5)
H12	0.0552	1.0919	0.6941	0.041*
C18	−0.4307 (3)	1.0377 (3)	0.5217 (3)	0.0327 (5)
H18	−0.4126	1.1284	0.5380	0.039*
C19	0.2159 (3)	0.5721 (3)	0.3699 (3)	0.0340 (6)
C20	0.2723 (3)	0.5366 (2)	0.2737 (2)	0.0275 (5)
C21	0.4203 (3)	0.5479 (3)	0.3167 (2)	0.0307 (5)
H21	0.4849	0.5687	0.4082	0.037*
C22	0.4726 (3)	0.5286 (3)	0.2259 (3)	0.0320 (5)
H22	0.5722	0.5378	0.2571	0.038*
C23	0.3784 (3)	0.4955 (2)	0.0874 (2)	0.0293 (5)
C24	0.2285 (3)	0.4760 (3)	0.0450 (3)	0.0362 (6)
H24	0.1622	0.4486	−0.0466	0.043*
C25	0.1767 (3)	0.4965 (3)	0.1363 (3)	0.0346 (6)
H25	0.0763	0.4833	0.1053	0.041*
C26	0.4304 (3)	0.4834 (3)	−0.0125 (3)	0.0336 (5)
H26	0.3584	0.4489	−0.1023	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02380 (10)	0.04032 (11)	0.02192 (9)	0.01038 (7)	0.01061 (7)	0.00110 (7)
O1	0.0278 (9)	0.0503 (12)	0.0424 (11)	0.0118 (9)	0.0134 (8)	0.0094 (9)
O1W	0.0276 (9)	0.0412 (11)	0.0387 (10)	0.0081 (8)	0.0165 (8)	0.0004 (8)
O2	0.0328 (10)	0.0434 (11)	0.0434 (11)	0.0182 (9)	0.0076 (9)	−0.0041 (9)
O3	0.0433 (11)	0.0654 (14)	0.0298 (10)	0.0133 (10)	0.0216 (9)	−0.0024 (9)
O4	0.0371 (12)	0.107 (2)	0.0525 (13)	0.0131 (13)	0.0317 (11)	−0.0010 (14)
N1	0.0301 (11)	0.0377 (12)	0.0269 (10)	0.0086 (9)	0.0120 (9)	0.0031 (9)

N2	0.0318 (11)	0.0385 (12)	0.0261 (10)	0.0087 (10)	0.0119 (9)	0.0050 (9)
C1	0.0362 (14)	0.0506 (17)	0.0383 (14)	0.0113 (13)	0.0200 (12)	0.0075 (13)
C2	0.0329 (15)	0.058 (2)	0.0551 (19)	0.0101 (14)	0.0222 (14)	0.0078 (16)
C3	0.0287 (14)	0.065 (2)	0.0487 (18)	0.0090 (14)	0.0082 (13)	0.0034 (16)
C4	0.0367 (15)	0.0524 (18)	0.0305 (14)	0.0118 (13)	0.0065 (12)	−0.0004 (13)
C5	0.0327 (13)	0.0297 (12)	0.0255 (11)	0.0112 (11)	0.0089 (10)	0.0035 (10)
C6	0.0368 (13)	0.0288 (12)	0.0230 (11)	0.0107 (11)	0.0124 (10)	0.0041 (9)
C7	0.0462 (16)	0.0462 (16)	0.0245 (12)	0.0081 (13)	0.0116 (12)	−0.0010 (12)
C8	0.067 (2)	0.0551 (19)	0.0290 (14)	0.0143 (17)	0.0279 (15)	0.0004 (13)
C9	0.0561 (19)	0.0530 (18)	0.0438 (16)	0.0145 (15)	0.0341 (15)	0.0085 (14)
C10	0.0366 (14)	0.0465 (16)	0.0376 (14)	0.0089 (13)	0.0192 (12)	0.0058 (12)
C11	0.0296 (13)	0.0454 (15)	0.0242 (11)	0.0159 (12)	0.0116 (10)	0.0063 (11)
C12	0.0280 (12)	0.0370 (13)	0.0294 (12)	0.0131 (11)	0.0139 (10)	0.0067 (10)
C13	0.0317 (14)	0.0350 (14)	0.0544 (17)	0.0127 (12)	0.0170 (13)	−0.0034 (13)
C14	0.0265 (13)	0.0371 (15)	0.0527 (17)	0.0080 (12)	0.0145 (12)	−0.0014 (13)
C15	0.0285 (12)	0.0368 (13)	0.0299 (12)	0.0140 (11)	0.0146 (10)	0.0110 (10)
C16	0.0356 (14)	0.0315 (13)	0.0356 (13)	0.0131 (11)	0.0149 (11)	0.0059 (11)
C17	0.0285 (12)	0.0362 (14)	0.0316 (13)	0.0092 (11)	0.0117 (11)	0.0046 (11)
C18	0.0326 (13)	0.0360 (14)	0.0307 (12)	0.0152 (11)	0.0143 (11)	0.0090 (10)
C19	0.0370 (14)	0.0363 (14)	0.0330 (13)	0.0058 (11)	0.0256 (12)	0.0026 (11)
C20	0.0303 (12)	0.0285 (12)	0.0269 (11)	0.0071 (10)	0.0191 (10)	0.0032 (9)
C21	0.0286 (12)	0.0361 (13)	0.0238 (11)	0.0079 (10)	0.0124 (10)	0.0025 (10)
C22	0.0269 (12)	0.0406 (14)	0.0309 (12)	0.0125 (11)	0.0168 (10)	0.0048 (11)
C23	0.0319 (12)	0.0328 (13)	0.0281 (12)	0.0110 (10)	0.0191 (10)	0.0060 (10)
C24	0.0312 (13)	0.0525 (17)	0.0236 (12)	0.0130 (12)	0.0137 (10)	0.0060 (11)
C25	0.0269 (12)	0.0508 (16)	0.0284 (12)	0.0128 (12)	0.0168 (11)	0.0064 (11)
C26	0.0345 (13)	0.0434 (15)	0.0270 (12)	0.0139 (12)	0.0187 (11)	0.0065 (11)

Geometric parameters (Å, º)

Cd1—O2	2.209 (2)	C9—H9	0.9300
Cd1—O1	2.745 (2)	C10—H10	0.9300
Cd1—O3	2.2129 (19)	C11—C12	1.506 (3)
Cd1—O1W	2.291 (2)	C12—C13	1.383 (4)
Cd1—N1	2.316 (3)	C12—C17	1.388 (4)
Cd1—N2	2.375 (2)	C13—C14	1.382 (4)
O1—C11	1.230 (3)	C13—H13	0.9300
O1W—H1W2	0.85 (4)	C14—C15	1.388 (4)
O1W—H1W1	0.850 (10)	C14—H15	0.9300
O2—C11	1.274 (3)	C15—C16	1.394 (4)
O3—C19	1.261 (3)	C15—C18	1.465 (3)
O4—C19	1.236 (3)	C16—C17	1.385 (4)
N1—C1	1.339 (4)	C16—H16	0.9300
N1—C5	1.348 (3)	C17—H12	0.9300
N2—C10	1.330 (4)	C18—C18^{i}	1.332 (5)
N2—C6	1.335 (3)	C18—H18	0.9300
C1—C2	1.377 (4)	C19—C20	1.496 (3)
C1—H1	0.9300	C20—C25	1.388 (3)

C2—C3	1.373 (5)	C20—C21	1.392 (3)
C2—H2	0.9300	C21—C22	1.377 (3)
C3—C4	1.373 (5)	C21—H21	0.9300
C3—H3	0.9300	C22—C23	1.399 (4)
C4—C5	1.386 (4)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.395 (4)
C5—C6	1.484 (4)	C23—C26	1.463 (3)
C6—C7	1.389 (4)	C24—C25	1.380 (3)
C7—C8	1.376 (5)	C24—H24	0.9300
C7—H7	0.9300	C25—H25	0.9300
C8—C9	1.373 (5)	C26—C26^{ii}	1.319 (5)
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.382 (4)		

O1—Cd1—O1W	139.33 (8)	C10—C9—H9	121.0
O1—Cd1—O2	51.29 (8)	N2—C10—C9	122.6 (3)
O1—Cd1—O3	120.67 (8)	N2—C10—H10	118.7
O1—Cd1—N1	94.47 (8)	C9—C10—H10	118.7
O1—Cd1—N2	74.71 (8)	O1—C11—O2	122.7 (2)
O2—Cd1—O3	115.76 (8)	O1—C11—C12	121.5 (2)
O2—Cd1—O1W	94.06 (8)	O2—C11—C12	115.8 (2)
O3—Cd1—O1W	91.48 (8)	C13—C12—C17	118.5 (2)
O2—Cd1—N1	144.70 (8)	C13—C12—C11	120.5 (2)
O3—Cd1—N1	87.35 (8)	C17—C12—C11	121.0 (2)
O1W—Cd1—N1	112.58 (8)	C14—C13—C12	120.8 (3)
O2—Cd1—N2	89.94 (8)	C14—C13—H13	119.6
O3—Cd1—N2	154.30 (8)	C12—C13—H13	119.6
O1W—Cd1—N2	86.30 (8)	C13—C14—C15	121.1 (3)
N1—Cd1—N2	70.07 (8)	C13—C14—H15	119.4
Cd1—O1—C11	80.8 (2)	C15—C14—H15	119.4
Cd1—O1W—H1W2	107 (2)	C14—C15—C16	118.0 (2)
Cd1—O1W—H1W1	116 (2)	C14—C15—C18	121.2 (2)
H1W2—O1W—H1W1	109.2 (16)	C16—C15—C18	120.8 (2)
C11—O2—Cd1	105.08 (17)	C17—C16—C15	120.7 (2)
C19—O3—Cd1	122.77 (18)	C17—C16—H16	119.6
C1—N1—C5	119.0 (2)	C15—C16—H16	119.6
C1—N1—Cd1	122.10 (18)	C16—C17—C12	120.8 (3)
C5—N1—Cd1	118.82 (18)	C16—C17—H12	119.6
C10—N2—C6	119.4 (2)	C12—C17—H12	119.6
C10—N2—Cd1	122.77 (19)	C18^{i}—C18—C15	125.8 (3)
C6—N2—Cd1	117.27 (17)	C18^{i}—C18—H18	117.1
N1—C1—C2	122.9 (3)	C15—C18—H18	117.1
N1—C1—H1	118.6	O4—C19—O3	124.5 (2)
C2—C1—H1	118.6	O4—C19—C20	118.2 (2)
C3—C2—C1	118.1 (3)	O3—C19—C20	117.2 (2)
C3—C2—H2	121.0	C25—C20—C21	118.0 (2)
C1—C2—H2	121.0	C25—C20—C19	119.7 (2)
C4—C3—C2	119.8 (3)	C21—C20—C19	122.3 (2)

C4—C3—H3	120.1	C22—C21—C20	121.1 (2)
C2—C3—H3	120.1	C22—C21—H21	119.5
C3—C4—C5	119.6 (3)	C20—C21—H21	119.5
C3—C4—H4	120.2	C21—C22—C23	121.1 (2)
C5—C4—H4	120.2	C21—C22—H22	119.4
N1—C5—C4	120.7 (3)	C23—C22—H22	119.4
N1—C5—C6	116.8 (2)	C24—C23—C22	117.4 (2)
C4—C5—C6	122.5 (2)	C24—C23—C26	119.5 (2)
N2—C6—C7	121.3 (3)	C22—C23—C26	123.1 (2)
N2—C6—C5	116.6 (2)	C25—C24—C23	121.3 (2)
C7—C6—C5	122.1 (3)	C25—C24—H24	119.4
C8—C7—C6	118.7 (3)	C23—C24—H24	119.4
C8—C7—H7	120.7	C24—C25—C20	120.9 (2)
C6—C7—H7	120.7	C24—C25—H25	119.5
C9—C8—C7	120.0 (3)	C20—C25—H25	119.5
C9—C8—H8	120.0	C26^{ii}—C26—C23	126.3 (3)
C7—C8—H8	120.0	C26^{ii}—C26—H26	116.8
C8—C9—C10	118.0 (3)	C23—C26—H26	116.8
C8—C9—H9	121.0		

O3—Cd1—O2—C11	−111.71 (18)	N2—C6—C7—C8	−0.1 (4)
O1W—Cd1—O2—C11	154.68 (18)	C5—C6—C7—C8	179.3 (3)
N1—Cd1—O2—C11	14.6 (3)	C6—C7—C8—C9	0.0 (5)
N2—Cd1—O2—C11	68.40 (18)	C7—C8—C9—C10	0.1 (5)
O2—Cd1—O3—C19	−22.1 (3)	C6—N2—C10—C9	−0.1 (4)
O1W—Cd1—O3—C19	73.1 (2)	Cd1—N2—C10—C9	−171.0 (2)
N1—Cd1—O3—C19	−174.3 (2)	C8—C9—C10—N2	0.0 (5)
N2—Cd1—O3—C19	157.7 (2)	Cd1—O2—C11—O1	3.9 (3)
O2—Cd1—N1—C1	−125.3 (2)	Cd1—O2—C11—C12	−174.36 (17)
O3—Cd1—N1—C1	8.2 (2)	O1—C11—C12—C13	176.0 (3)
O1W—Cd1—N1—C1	98.7 (2)	O2—C11—C12—C13	−5.6 (4)
N2—Cd1—N1—C1	175.6 (2)	O1—C11—C12—C17	−1.5 (4)
O2—Cd1—N1—C5	58.1 (3)	O2—C11—C12—C17	176.8 (2)
O3—Cd1—N1—C5	−168.5 (2)	C17—C12—C13—C14	−1.0 (5)
O1W—Cd1—N1—C5	−78.0 (2)	C11—C12—C13—C14	−178.7 (3)
N2—Cd1—N1—C5	−1.02 (18)	C12—C13—C14—C15	−0.7 (5)
O2—Cd1—N2—C10	25.7 (2)	C13—C14—C15—C16	1.3 (4)
O3—Cd1—N2—C10	−154.1 (2)	C13—C14—C15—C18	−178.7 (3)
O1W—Cd1—N2—C10	−68.4 (2)	C14—C15—C16—C17	−0.2 (4)
N1—Cd1—N2—C10	176.0 (2)	C18—C15—C16—C17	179.8 (2)
O2—Cd1—N2—C6	−145.44 (19)	C15—C16—C17—C12	−1.5 (4)
O3—Cd1—N2—C6	34.8 (3)	C13—C12—C17—C16	2.1 (4)
O1W—Cd1—N2—C6	120.49 (19)	C11—C12—C17—C16	179.8 (2)
N1—Cd1—N2—C6	4.85 (18)	C14—C15—C18—C18^{i}	16.2 (5)
C5—N1—C1—C2	−0.4 (4)	C16—C15—C18—C18^{i}	−163.8 (3)
Cd1—N1—C1—C2	−177.1 (2)	Cd1—O3—C19—O4	3.1 (4)
N1—C1—C2—C3	0.0 (5)	Cd1—O3—C19—C20	178.25 (17)
C1—C2—C3—C4	−0.2 (5)	O4—C19—C20—C25	5.7 (4)

C2—C3—C4—C5	0.8 (5)	O3—C19—C20—C25	−169.8 (3)
C1—N1—C5—C4	1.0 (4)	O4—C19—C20—C21	−177.2 (3)
Cd1—N1—C5—C4	177.7 (2)	O3—C19—C20—C21	7.3 (4)
C1—N1—C5—C6	−179.3 (2)	C25—C20—C21—C22	4.4 (4)
Cd1—N1—C5—C6	−2.5 (3)	C19—C20—C21—C22	−172.8 (2)
C3—C4—C5—N1	−1.2 (5)	C20—C21—C22—C23	−0.8 (4)
C3—C4—C5—C6	179.1 (3)	C21—C22—C23—C24	−3.3 (4)
C10—N2—C6—C7	0.1 (4)	C21—C22—C23—C26	175.4 (3)
Cd1—N2—C6—C7	171.6 (2)	C22—C23—C24—C25	3.9 (4)
C10—N2—C6—C5	−179.3 (2)	C26—C23—C24—C25	−174.9 (3)
Cd1—N2—C6—C5	−7.8 (3)	C23—C24—C25—C20	−0.4 (4)
N1—C5—C6—N2	6.9 (3)	C21—C20—C25—C24	−3.8 (4)
C4—C5—C6—N2	−173.3 (3)	C19—C20—C25—C24	173.5 (3)
N1—C5—C6—C7	−172.5 (3)	C24—C23—C26—C26^{ii}	169.8 (4)
C4—C5—C6—C7	7.3 (4)	C22—C23—C26—C26^{ii}	−8.9 (5)

Symmetry codes: (i) −*x*−1, −*y*+2, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{iii}	0.85 (1)	1.92 (2)	2.697 (3)	152 (3)
O1*W*—H1*W*2···O4^{iii}	0.85 (4)	1.81 (4)	2.639 (3)	167 (3)

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