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Poly[diaqua-1κ^2*O*-bis[μ_3-2-(1*H*-tetrazol-5-yl)benzoato(2−)]dicadmium(II)]

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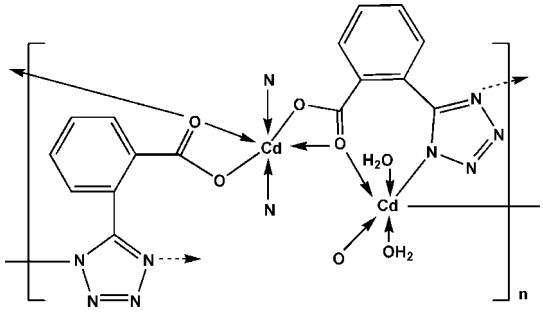
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.046; data-to-parameter ratio = 12.7.

The title compound, $[Cd_2(C_8H_4N_4O_2)_2(H_2O)_2]_n$, is a coordination polymer prepared by the hydrothermal reaction of cadmium(II) chloride and 2-(1*H*-tetrazol-5-yl)benzoic acid. Two types of coordinated cadmium cations exist in the structure. One is located on a twofold axis and is coordinated by four O and two N atoms from four symmetry-related ligands, forming a trigonal-prismatic coordination polyhedron. The other is located on an inversion center and is octahedrally coordinated by two N and two O atoms from two ligands in equatorial sites, and two water molecules in axial sites. The organic ligand bridges three Cd atoms, through a carboxylate group and two N atoms of the tetrazolate unit. This mode of coordination results in a two-dimensional framework. The crystal structure is stabilized by intermolecular O—H···O and O—H···N hydrogen bonds.

Related literature

For the chemistry of tetrazole derivatives, see: Xiong *et al.* (2002); Xue *et al.* (2002); Dunica *et al.* (1991); Wang *et al.* (2005); Wittenberger *et al.* (1993); Hu *et al.* (2007).



Experimental

Crystal data

$[Cd_2(C_8H_4N_4O_2)_2(H_2O)_2]$
M_r = 637.16
Monoclinic, $C2/c$
a = 19.886 (4) Å
b = 7.3522 (15) Å
c = 15.409 (3) Å
β = 115.97 (3)°
V = 2025.4 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.15 mm^{-1}
T = 293 (2) K
0.35 × 0.30 × 0.10 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.473, T_{max} = 0.809
8913 measured reflections
1976 independent reflections
1922 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.046
S = 1.13
1976 reflections
156 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O2^{i}	0.75 (4)	2.06 (4)	2.758 (2)	156 (4)
O1W—H2W···N2^{ii}	0.87 (4)	2.14 (4)	2.961 (3)	155 (3)

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *PRPKAPPA* (Ferguson, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2178).

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supplementary materials

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Poly[diaqua-1κ^2O-bis[μ_3-2-(1*H*-tetrazol-5-yl)benzoato(2-)]dicadmium(II)]

X.-Z. Li, B.-Z. Wu and Z.-R. Qu

Comment

Coordination frameworks have received much attention over the past decade because of their potential applications. Multi-functional organic ligands are necessary to construct such frameworks. 2-(1*H*-tetrazol-5-yl)benzoic acid is a ligand with two functional groups, one carboxylate group and one tetrazole ring. Tetrazole compounds have a wide range of applications in coordination chemistry, medicinal chemistry and material science (Hu *et al.*, 2007; Xiong *et al.*, 2002; Xue *et al.*, 2002; Wang *et al.*, 2005; Dunica *et al.*, 1991; Wittenberger *et al.*, 1993). We report here the crystal structure of the title compound, which was obtained by the hydrothermal reaction of cadmium chloride and 2-(1*H*-tetrazol-5-yl)benzoic acid.

In the structure of this compound, two types of coordinated cadmium cations exist (Fig. 1). Cd1 is located on a 2-fold rotation axis, and is trigonal prismatically coordinated by two O and two N from four different ligands. While Cd2 is loacated on an inversion center, and is octahedrally coordinated by two N and two O from two ligands at equatorial sites, and two O atoms of H_2O at axial sites. The organic ligand bridges three Cd atoms by coordinating one Cd atom through one N atom from the tetrazole unit, by coordinating the other Cd atom through one O atom and one μ_3-O from the carboxylate unit, and by coordinating a third Cd atom through a N atom from the tetrazole unit and one μ_3-O from the carboxylate unit. Such an arrangement makes Cd1 and Cd2 bridged by one μ_3-O carboxylate group and the tetrazole unit, resulting in a two-dimensional framework (Fig. 2). The crystal structure is stabilized by intermolecular O—H···O and O—H···N hydrogen bonds (Table 1).

Experimental

A mixture of $CdCl_2$ (0.2 mmol) and 2-(1*H*-tetrazol-5-yl)benzoic acid (0.2 mmol) in H_2O (4 ml) was heated in a Pyrex tube at 373 K for two days. After slowly cooling down to room temperature over a period of 12 h., colourless crystals of the title compound suitable for diffraction were isolated.

Refinement

Water H atoms were found in a difference map and refined freely. Other H atoms positions were calculated geometrically and these H atoms were allowed to ride on their carrier C atoms with C—H = 0.93 Å, and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

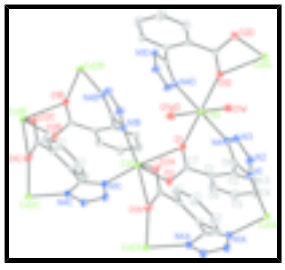


Fig. 1. A partial packing diagram of the title compound, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) *-x, -y + 1, -z*; (B) *-x, +y, 1/2 - z*; (C) *+x, +y - 1, +z*; (D) *-x, +y - 1, 1/2 - z*.]

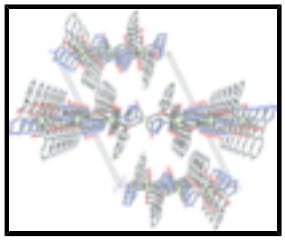


Fig. 2. Packing diagram of the title compound, showing the structure along the *b* axis. No displacement parameters are displayed and H atoms have been omitted for clarity.

(I)

Crystal data

$[Cd_2(C_8H_4N_4O_2)_2(H_2O)_2]$	F_{000} = 1232
M_r = 637.16	D_x = 2.090 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 0 reflections
a = 19.886 (4) Å	θ = 3.1–27.5º
b = 7.3522 (15) Å	μ = 2.15 mm^{-1}
c = 15.409 (3) Å	*T* = 293 (2) K
β = 115.97 (3)º	Block, colourless
V = 2025.4 (7) Å^3	0.35 × 0.30 × 0.10 mm
Z = 4	

Data collection

Rigaku SCXmini diffractometer	1976 independent reflections
Radiation source: fine-focus sealed tube	1922 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
Detector resolution: 13.6612 pixels mm^{-1}	θ_{max} = 26.0º
T = 293(2) K	θ_{min} = 3.0º
CCD Profile fitting scans	*h* = −24→24
Absorption correction: multi-scan (CrystalClear; Rigaku, 2005)	*k* = −9→9
T_{min} = 0.473, T_{max} = 0.809	*l* = −18→18
8913 measured reflections	

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.046$

$S = 1.13$

1976 reflections

156 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0214P)^2 + 3.1517P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.36$ e Å^{-3}

$\Delta\rho_{min} = -0.42$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00235 (14)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.0000	0.21274 (3)	0.2500	0.02355 (9)
Cd2	0.0000	0.5000	0.0000	0.02567 (9)
O1	0.05131 (10)	0.4374 (2)	0.16197 (11)	0.0376 (4)
O1W	0.11318 (10)	0.6113 (3)	0.00533 (13)	0.0352 (4)
H1W	0.115 (2)	0.579 (5)	−0.040 (3)	0.063 (11)*
H2W	0.115 (2)	0.730 (6)	0.006 (3)	0.071 (11)*
O2	0.09395 (10)	0.4136 (2)	0.31727 (11)	0.0361 (4)
N1	−0.01798 (10)	1.0095 (2)	0.13491 (13)	0.0239 (4)
N2	−0.08259 (11)	1.0024 (2)	0.05335 (14)	0.0303 (4)
N3	−0.08190 (11)	0.8588 (3)	0.00480 (13)	0.0319 (4)
N4	−0.01705 (10)	0.7689 (2)	0.05357 (13)	0.0264 (4)
C1	0.12913 (12)	0.6784 (3)	0.26098 (15)	0.0235 (4)
C2	0.09950 (11)	0.8385 (3)	0.20847 (14)	0.0223 (4)
C3	0.14406 (14)	0.9941 (3)	0.23224 (17)	0.0308 (5)
H3	0.1253	1.1003	0.1971	0.037*
C4	0.21556 (14)	0.9938 (3)	0.3061 (2)	0.0409 (6)
H4	0.2444	1.0989	0.3208	0.049*
C5	0.24392 (14)	0.8370 (4)	0.3581 (2)	0.0450 (6)
H5	0.2921	0.8361	0.4082	0.054*
C6	0.20091 (13)	0.6821 (3)	0.33610 (17)	0.0361 (5)
H6	0.2203	0.5772	0.3722	0.043*
C7	0.08845 (12)	0.5008 (3)	0.24438 (16)	0.0225 (4)
C8	0.02201 (11)	0.8642 (3)	0.13370 (14)	0.0204 (4)

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cd1	0.03345 (14)	0.01501 (12)	0.01947 (13)	0.000	0.00909 (9)	0.000
Cd2	0.03771 (15)	0.01834 (13)	0.01698 (13)	0.00252 (8)	0.00830 (10)	−0.00369 (7)
O1	0.0559 (11)	0.0246 (8)	0.0209 (8)	−0.0100 (8)	0.0062 (7)	−0.0002 (6)
O1W	0.0392 (10)	0.0341 (10)	0.0287 (9)	0.0054 (7)	0.0116 (7)	0.0008 (7)
O2	0.0511 (10)	0.0304 (9)	0.0210 (7)	−0.0135 (8)	0.0105 (7)	0.0019 (6)
N1	0.0276 (9)	0.0179 (8)	0.0205 (9)	0.0017 (7)	0.0052 (7)	−0.0029 (6)
N2	0.0298 (10)	0.0247 (10)	0.0277 (10)	0.0045 (7)	0.0047 (8)	−0.0028 (7)
N3	0.0328 (10)	0.0261 (10)	0.0259 (9)	0.0037 (8)	0.0028 (8)	−0.0050 (8)
N4	0.0298 (9)	0.0218 (9)	0.0214 (9)	0.0027 (7)	0.0053 (7)	−0.0048 (7)
C1	0.0256 (10)	0.0215 (10)	0.0223 (10)	−0.0005 (8)	0.0095 (8)	−0.0014 (8)
C2	0.0256 (10)	0.0211 (10)	0.0204 (10)	−0.0008 (8)	0.0102 (8)	−0.0019 (8)
C3	0.0334 (13)	0.0233 (11)	0.0325 (13)	−0.0042 (9)	0.0113 (10)	0.0011 (8)
C4	0.0319 (13)	0.0332 (13)	0.0482 (16)	−0.0132 (10)	0.0090 (11)	−0.0041 (10)
C5	0.0262 (12)	0.0430 (14)	0.0456 (15)	−0.0062 (11)	−0.0029 (10)	0.0007 (12)
C6	0.0295 (12)	0.0306 (12)	0.0352 (13)	0.0011 (10)	0.0022 (10)	0.0063 (10)
C7	0.0242 (11)	0.0199 (10)	0.0212 (11)	0.0029 (7)	0.0077 (9)	0.0006 (7)
C8	0.0264 (10)	0.0156 (9)	0.0195 (9)	−0.0017 (8)	0.0102 (8)	−0.0010 (7)

Geometric parameters (Å, °)

Cd1—N1^{i}	2.2251 (17)	N1—N2	1.349 (3)
Cd1—N1^{ii}	2.2251 (17)	N1—Cd1^{v}	2.2251 (17)
Cd1—O2	2.2473 (16)	N2—N3	1.298 (3)
Cd1—O2^{iii}	2.2473 (16)	N3—N4	1.347 (3)
Cd1—O1	2.6117 (17)	N4—C8	1.333 (3)
Cd1—O1^{iii}	2.6118 (17)	C1—C6	1.390 (3)
Cd1—C7^{iii}	2.779 (2)	C1—C2	1.404 (3)
Cd2—N4^{iv}	2.2251 (18)	C1—C7	1.498 (3)
Cd2—N4	2.2251 (18)	C2—C3	1.394 (3)
Cd2—O1	2.2916 (16)	C2—C8	1.477 (3)
Cd2—O1^{iv}	2.2916 (16)	C3—C4	1.378 (4)
Cd2—O1W	2.3623 (19)	C3—H3	0.9300
Cd2—O1W^{iv}	2.3623 (19)	C4—C5	1.376 (4)
O1—C7	1.247 (3)	C4—H4	0.9300
O1W—H1W	0.75 (4)	C5—C6	1.375 (3)
O1W—H2W	0.87 (4)	C5—H5	0.9300
O2—C7	1.256 (3)	C6—H6	0.9300
N1—C8	1.337 (3)		
N1^{i}—Cd1—N1^{ii}	95.61 (9)	Cd2—O1—Cd1	127.14 (7)
N1^{i}—Cd1—O2	128.32 (7)	Cd2—O1W—H1W	107 (3)
N1^{ii}—Cd1—O2	105.23 (6)	Cd2—O1W—H2W	112 (2)
N1^{i}—Cd1—O2^{iii}	105.23 (6)	H1W—O1W—H2W	108 (4)
N1^{ii}—Cd1—O2^{iii}	128.32 (7)	C7—O2—Cd1	101.17 (13)
O2—Cd1—O2^{iii}	97.83 (9)	C8—N1—N2	106.63 (16)
N1^{i}—Cd1—O1	88.50 (6)	C8—N1—Cd1^{v}	131.21 (14)
N1^{ii}—Cd1—O1	151.13 (6)	N2—N1—Cd1^{v}	121.56 (13)

O2—Cd1—O1	52.34 (5)	N3—N2—N1	108.79 (17)
O2^{iii}—Cd1—O1	77.28 (6)	N2—N3—N4	109.07 (17)
N1^{i}—Cd1—O1^{iii}	151.13 (6)	C8—N4—N3	106.63 (17)
N1^{ii}—Cd1—O1^{iii}	88.50 (6)	C8—N4—Cd2	133.51 (14)
O2—Cd1—O1^{iii}	77.28 (6)	N3—N4—Cd2	119.53 (13)
O2^{iii}—Cd1—O1^{iii}	52.34 (5)	C6—C1—C2	118.9 (2)
O1—Cd1—O1^{iii}	101.55 (8)	C6—C1—C7	116.11 (19)
N1^{i}—Cd1—C7^{iii}	130.83 (7)	C2—C1—C7	125.01 (19)
N1^{ii}—Cd1—C7^{iii}	111.72 (7)	C3—C2—C1	118.60 (19)
O2—Cd1—C7^{iii}	83.94 (7)	C3—C2—C8	115.22 (19)
O2^{iii}—Cd1—C7^{iii}	26.32 (6)	C1—C2—C8	126.00 (18)
O1—Cd1—C7^{iii}	86.03 (6)	C4—C3—C2	121.5 (2)
O1^{iii}—Cd1—C7^{iii}	26.51 (6)	C4—C3—H3	119.2
N4^{iv}—Cd2—N4	180.00 (10)	C2—C3—H3	119.3
N4^{iv}—Cd2—O1	99.09 (6)	C5—C4—C3	119.6 (2)
N4—Cd2—O1	80.91 (6)	C5—C4—H4	120.2
N4^{iv}—Cd2—O1^{iv}	80.91 (6)	C3—C4—H4	120.2
N4—Cd2—O1^{iv}	99.09 (6)	C6—C5—C4	119.9 (2)
O1—Cd2—O1^{iv}	180.0	C6—C5—H5	120.1
N4^{iv}—Cd2—O1W	91.33 (7)	C4—C5—H5	120.0
N4—Cd2—O1W	88.67 (7)	C5—C6—C1	121.5 (2)
O1—Cd2—O1W	93.94 (7)	C5—C6—H6	119.3
O1^{iv}—Cd2—O1W	86.06 (7)	C1—C6—H6	119.2
N4^{iv}—Cd2—O1W^{iv}	88.67 (7)	O1—C7—O2	120.06 (19)
N4—Cd2—O1W^{iv}	91.33 (7)	O1—C7—C1	122.33 (19)
O1—Cd2—O1W^{iv}	86.06 (7)	O2—C7—C1	117.60 (19)
O1^{iv}—Cd2—O1W^{iv}	93.94 (7)	N4—C8—N1	108.88 (18)
O1W—Cd2—O1W^{iv}	180.00 (9)	N4—C8—C2	129.86 (18)
C7—O1—Cd2	144.77 (14)	N1—C8—C2	120.98 (17)
C7—O1—Cd1	84.22 (13)		

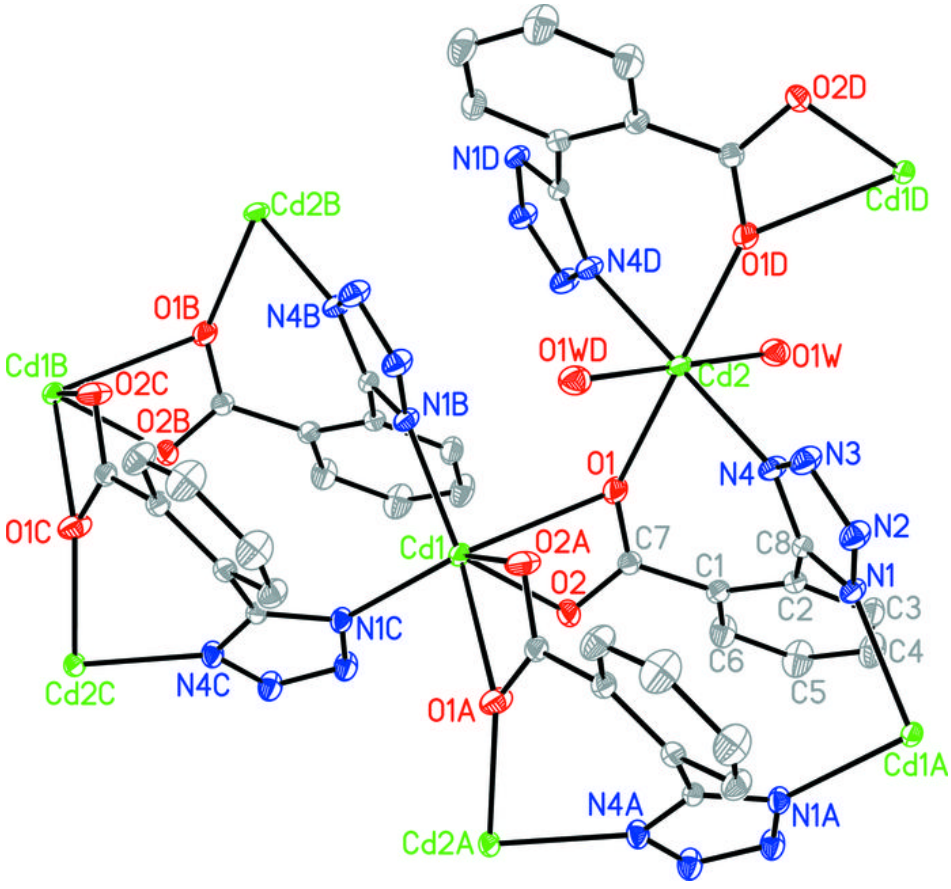
Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*, *y*−1, −*z*+1/2; (iii) −*x*, *y*, −*z*+1/2; (iv) −*x*, −*y*+1, −*z*; (v) *x*, *y*+1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W···O2^{vi}	0.75 (4)	2.06 (4)	2.758 (2)	156 (4)
O1W—H2W···N2^{vii}	0.87 (4)	2.14 (4)	2.961 (3)	155 (3)

Symmetry codes: (vi) *x*, −*y*+1, *z*−1/2; (vii) −*x*, −*y*+2, −*z*.

Fig. 1


O2D
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Cd1D
Cd2B
N4D
O1D
O1B
N4B
O1WD
O1W
Cd1B
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N1B
O2B
O1
N4
N3
O1C
Cd1
O2A
C7
C8
N2
C1
O2
N1
C2
C3
N1C
C6
C4
C5
Cd2C
N4C
O1A
Cd1A
N4A
N1A
Cd2A

Fig. 2